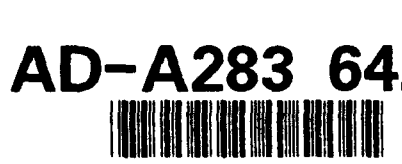

ARMY RESEARCH LABORATORY

Preparation and Extension of the Thermodynamics Program BLAKE and Its Library to 10,000 K for Use With Electrothermal-Chemical (ETC) Systems

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U.S. ARMY RESEARCH LABORATORY

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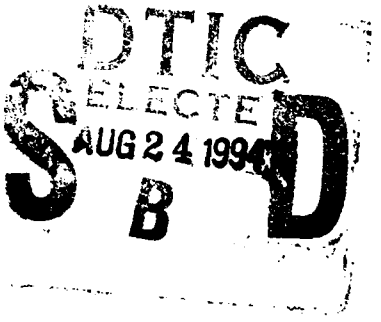
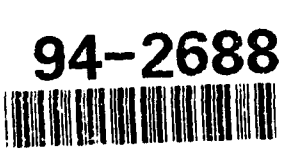
ARL-TR-488 July 1994





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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	July 1994	Final, October 1992–October 1993

4. TITLE AND SUBTITLE

Preparation and Extension of The Thermodynamics Program BLAKE and Its Library to 10,000 K for Use With Electrothermal-Chemical (ETC) Systems

5. FUNDING NUMBERS

PR: 1L162618A1FL

6. AUTHOR(S)

William Oberle (U.S. Army Research Laboratory) and Eli Freedman (Eli Freedman & Associates)

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

U.S. Army Research Laboratory
ATTN: AMSRL-WT-PA
Aberdeen Proving Ground, MD 21005-5066

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U.S. Army Research Laboratory
ATTN: AMSRL-OP-AP-L
Aberdeen Proving Ground, MD 21005-5066

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

ARL-TR-488

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

This report reviews the rationale for the selection of the BLAKE thermochemical code as the basis for an extended thermochemical code for use with electrothermal-chemical (ETC) plasma/propellants mixtures. Basically, it is shown that the formation of ions in the propellant gases at temperatures created by the introduction of an electrically generated plasma does not significantly change the calculated thermochemical values. No modification is therefore required for BLAKE; all that had to be done was to create a new library containing data covering the temperature range up to 10,000 K for the majority of species occurring in the ETC propulsion process. Users choose the desired library (standard or extended) just prior to running the program. The report concludes with results of test cases illustrating effects due to the use of thermochemical data for the extended temperature range.

14. SUBJECT TERMS

propellants, thermochemical properties, ballistics, electrothermal-chemical

15. NUMBER OF PAGES

132

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

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1. INTRODUCTION AND STATEMENT OF THE PROBLEM

The evaluation of the potential performance of gas-driven gun propulsion concepts requires an accurate determination of the thermochemical properties of the propelling gases. The principal quantities of interest are as follows: (1) the effective gas temperature (flame temperature in the absence of electrical energy); (2) the ratio of the frozen specific heats (γ); (3) the covolume; and (4) the ballistic energy, which is defined by

$$\text{Ballistic Energy} = \frac{\text{impetus}}{\gamma - 1} . \tag{1}$$

Thermochemical codes designed for ballistic applications (i.e., utilizing nonideal equations of state) such as BLAKE (Freedman 1982), F. Volk's ICT code (Volk and Bathelt 1978), or SNPE's BAGHEERA (Kotlar 1991) have proven very effective in calculating these quantities for standard solid propellant gun systems. Unfortunately, calculating thermochemical values for gases produced by the plasma/propellant mixture in the electrothermal-chemical (ETC) ballistic process is complicated by the likelihood of achieving gas temperatures well in excess of 5,000 K.

Two potential difficulties, which can result in incorrect thermochemical values being calculated, arise when the gas temperature greatly exceeds 5,000 K. First, a significant concentration of ions may be formed in the gas at these temperatures; in their present forms, neither BLAKE nor the ICT code takes into account the presence of ions and their concomitant effect on the thermodynamics.

Second, the representations of the temperature dependence of the thermodynamic data used by the codes in performing the calculations may not be valid much beyond this temperature. This point requires further discussion. General-purpose thermodynamics codes, such as the ones mentioned, must have available as functions of temperature the thermodynamic quantities, heat capacity at constant pressure (C_p), enthalpy (H), and entropy (S), for 500–1,000 species. In order to minimize computer memory requirements, these quantities are not themselves stored directly. Since H and S are directly obtained by integration of $C_p(T)dT$ and $[C_p/T]dT$, respectively, it is sufficient to store only C_p plus two integration constants. Furthermore, even C_p itself is not stored directly; instead, the coefficients of an empirical representation are used.

There is no objective way of deciding which representation is the best. Gordon and McBride (1971) used

$$C_p(T)/\Re = c + d*T + e*T^2 + f*T^3 + g*T^4 . \quad (2)$$

More recently, McBride (1992) has been using

$$C_p(T)/\Re = a*T^{-2} + b*T^{-1} + c + d*T + e*T^2 + f*T^3 + g*T^4 . \quad (3)$$

The authors of the TIGER code (Cowperthwaite and Zwisler 1973), and subsequently, BLAKE, used

$$C_p(T)/\Re = B(1) + B(2)*\Theta + B(3)*\Theta^2 + B(4)*\Theta^3 + B(5)*(1/\Theta) + B(6)*(1/\Theta)^2 + B(7)*(1/\Theta)^3 . \quad (4)$$

In Eqs. 2–4, T is the absolute temperature and $\Re$ is the universal gas constant in appropriate units (originally, calories/mole-K; more recently, joules/mole-K). In Eq. (4), Θ is T/1,000.

In all cases, the constants a–g or B(1)–B(7) are determined by linear least squares fitting to the heat capacity data in the JANAF Tables (Chase et al. 1986). Earlier editions of the JANAF Tables terminated at 5,000 K and, therefore, so did the fittings in BLAKE and the ICT programs. Extrapolating linear least squares fittings is known to be a risky procedure. (This difficulty can often be avoided [Chase 1985] by including an estimated heat capacity at a temperature well outside the upper range, but this was not done in the BLAKE fittings.) Any inaccuracies arising from such extrapolation will be propagated through the calculations, possibly resulting in significant errors in the values determined for the other thermochemical properties.

Even when the total amount of added electrical energy is relatively low so that the overall average gas temperature remains below 5,000 K, transient high gas temperatures (over 5,000 K) with their (possibly) resulting inaccurate thermochemical properties may occur. (The time scale of these transients, while short compared to the gun firing cycle, is nevertheless long enough so that thermochemical equilibrium is maintained in the chamber.) This is illustrated in Figures 1 and 2. Figure 1 shows the calculated instantaneous electrical energy density (kilojoules of input electrical energy per gram of propellant consumed) for an experimental 30-mm ETC gun firing. One sees electrical energy densities

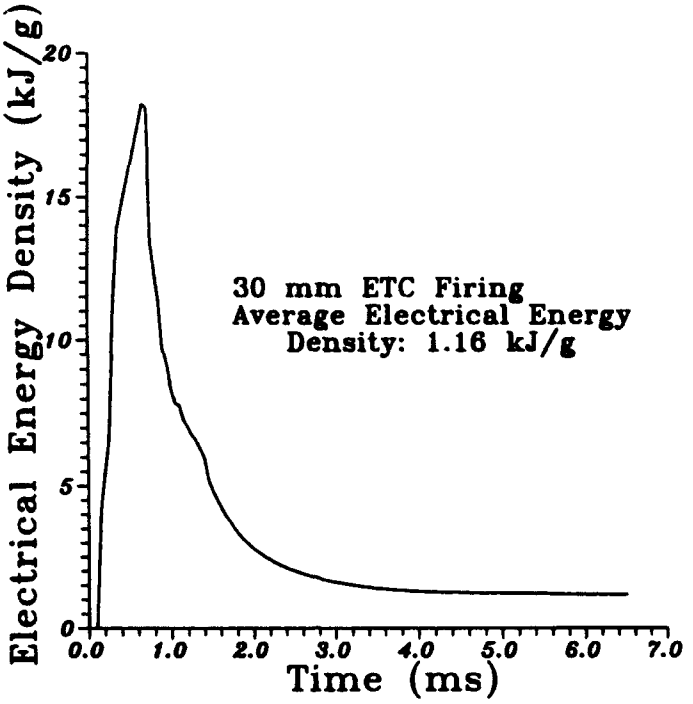

Figure 1. Instantaneous electrical energy density; 30-mm ETC gun firing.

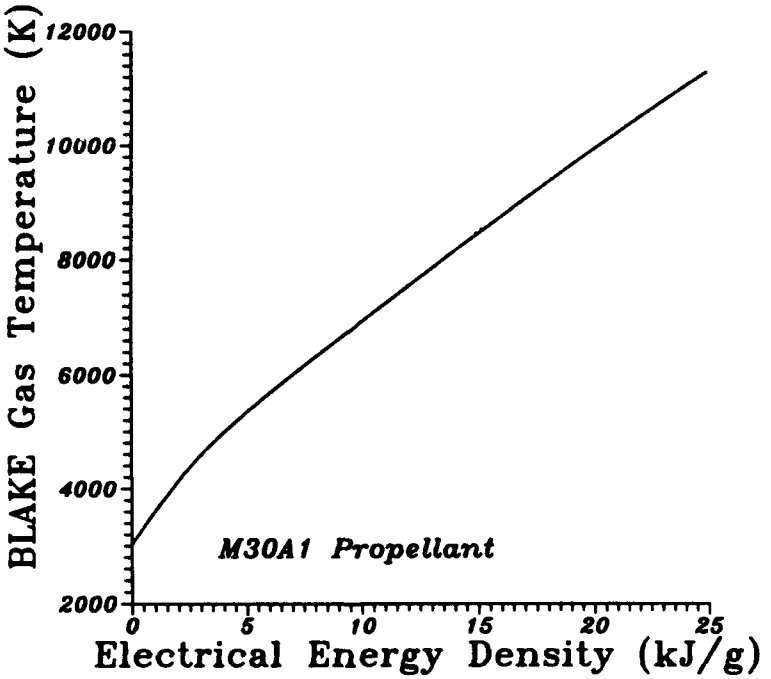

Figure 2. Computed gas temperature for firing of Figure 1.

greater than five occurring for about 1.2 ms during the first 1.4 ms of the ballistic cycle. Figure 2 shows that electrical energy densities greater than five (for the M30 propellant used in the experiment) result in calculated gas temperatures in excess of 5,000 K. Thus, even though the average plasma/propellant gas temperature is approximately 3,800 K (using an average electrical energy density of 1.16 kJ/g) during a significant portion of the ballistic cycle (1.2 ms of the total 6.4 ms, Figure 1), the effective gas temperature would exceed 5,000 K. Wren and Oberle (1993) have shown that ignoring the effects associated with the high transient gas temperatures and varying thermochemical properties can result in significant differences in interior ballistic simulations and in inverse analyses of experimental data for ETC systems.

The objective of the present work was to produce a unified thermodynamics code and its accompanying library that can produce all of the customary ballistic thermochemical data for ETC propellant systems at temperatures up to 10,000 K and preferably 15,000 K. Specifically discussed are the following: (1) the overall approach and rationale to producing the desired thermochemical code; (2) evaluation of the effect of including ions on calculated thermochemical values; (3) modifications to the BLAKE thermodynamics code; and (4) results of several test cases utilizing the unified thermochemical code with libraries over different temperature ranges.

2. APPROACH

In order to achieve the desired objectives, the following steps were adopted: (1) determine if the presence of ions at high temperatures significantly affects values for computed thermochemical data; (2) based upon the results of (1), decide which thermodynamic code to modify; and (3) modify the selected code.

2.1 Discussion of Step 1. To determine the potential effect of ions, the National Aeronautics and Space Administration Lewis Research Center's (NASA-Lewis) family of codes (CET86, TRAN72, CET89, and variants) (Gordon and McBride 1971; Svehla and McBride 1973) was selected for use since they can easily work with ions. Before evaluating the effect that ions may have on the computed thermochemical properties, however, it was necessary to obtain thermodynamic data for species produced in typical ETC gun propellants up to 10,000 K. Fortunately, Bonnie J. McBride of NASA-Lewis in Cleveland, OH, was able to provide to the Army Research Laboratory a set of coefficients that would permit computations up to 15,000 K (and 20,000 K in some cases) for 133 neutral and ionic species containing C-H-O-N.

Since ballistic energy (defined earlier) is the quantity actually utilized in most ballistic simulations, it was selected as the figure of merit for ascertaining the effect of ions. A difference of more than 2% in computed ballistic energy (with and without the formation of ions permitted) was selected as the decision criterion. Results are presented in the next section.

2.2 Discussion of Step 2. We consider only two codes, BLAKE and CET86, the next-to-latest version of the NASA's Lewis Research Center's chemical equilibrium and transport codes. Each code has its own advantages and disadvantages. CET86 is an outstanding program that is easy to run and readily works with ions. Unfortunately, it utilizes only the ideal gas equation and, therefore, cannot estimate covolumes, a necessity for gun calculations. If inclusion of ions proved to be necessary, then the CET86 code would be adopted, and a modification or separate program would be developed to compute covolumes. On the other hand, if the formation of ions is not significant at temperatures up to 10,000 K, then the BLAKE code would be used, and an extended library (valid up to at least 10,000 K) would be prepared for it.

2.3 Discussion of Step 3. As will be shown, the formation of ions was found not to be important (at least for the propellant systems considered), and consequently the BLAKE code was selected. Only a summary of the modifications to BLAKE will be provided in this report; more detailed information will be contained in a forthcoming report.

3. EFFECT OF IONS

As mentioned previously, the NASA-Lewis code CET86 was utilized to determine the effect of ions on the calculated thermochemical data. A variant of CET86 called MuCET* was chosen for this task. Unfortunately, the format of McBride's high-temperature thermochemical data differed from that used in all NASA-Lewis thermochemistry programs through CET89 and, hence, MuCET. It was therefore necessary to produce a modified version of MuCET to accommodate the new format for the high-temperature thermochemical data; this modified version of MuCET was named EXMuCET. Comparisons between MuCET and EXMuCET at temperatures below 5,000 K, using the same thermochemical library, were performed to ensure the accuracy of EXMuCET. Overall, the comparisons were excellent, but small differences in computed values were observed at temperatures below about

* MuCET is a version of NASA's CET86 adapted for easy use with IBM-compatible desktop computers. It was produced by Eli Freedman & Associates and is licensed to the U.S. Army.

3,000 K; these were caused by the occurrence or nonoccurrence of condensed phases. Since EXMuCET is intended for use primarily for temperatures above 5,000 K, the differences associated with inclusion or noninclusion of condensed phases are not considered important; their presence is ignored in all of the subsequent comparisons discussed here. Some standard propellants (e.g., M30) contain inorganic additives that result in the formation of condensed phases at chamber conditions. When necessary, these formulations have had such additives deleted from their compositions when entered into the codes; they are referred to as pseudopropellants. Additional details can be found in the appendix.

To determine the importance of ions on the thermodynamic calculations, eight propellant systems (listed in Table 1) were investigated with the formation of ions both permitted and forbidden over a wide range of electrical energy inputs, which produced computed temperatures in excess of 13,500 K.

Table 1. Propellant Systems Investigated With and Without Ions Permitted

1. Pseudo M30
2. WC890
3. JA2
4. M9
5. M1
6. Decalin + white fuming nitric acid
7. Decalin + 70% H_2O_2
8. Red fuming nitric acid + unsymmetrical dimethyl hydrazine

The differences in ballistic energies for the two conditions (ions included vs. no ions included) for pseudo-M30 and JA2 over a wide range of electrical energy densities (kilojoules of electrical energy added per gram of propellant) are shown in Figure 3. This figure shows that there is virtually no difference up to 10,000 K (solid square), corresponding to electrical energy densities of 22–23 kJ/g. The results are similar for the other six propellant systems investigated. The maximum percent differences in ballistic energy for the eight propellant systems at each electrical energy density (the propellant system producing the maximum percent difference may differ at each electrical energy density) are displayed in Figure 4. (See Appendix G of the overall appendix for details on all eight propellant systems.) As would be expected, this curve is similar in appearance to the ballistic energy difference curve of Figure 3.

In fact, for temperatures approaching 12,000 K (electrical energy density of 34 kJ/g), the maximum percent difference is less than 1.0%. Thus, based upon the criteria stated in the previous section, the

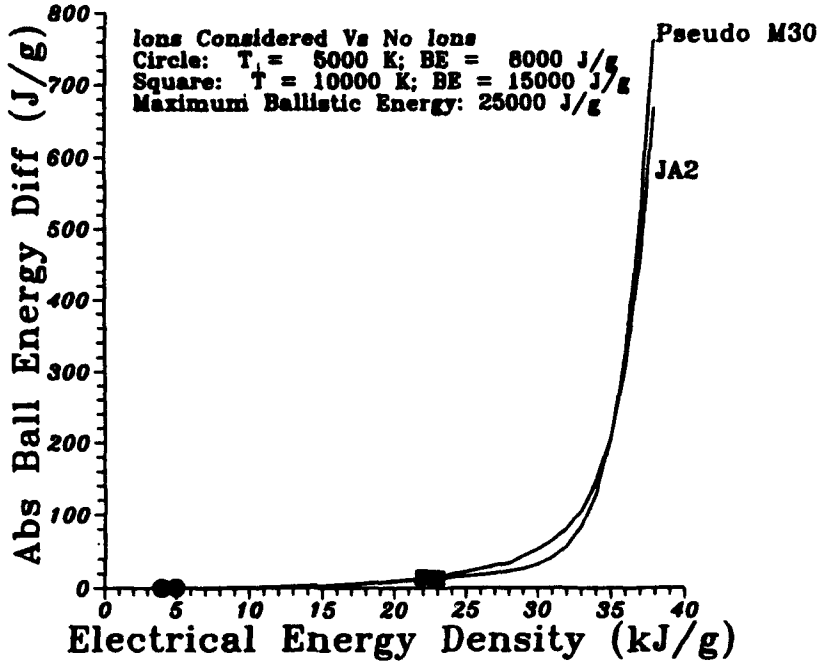

Figure 3. Difference in ballistic energies for M30 and JA2 propellants with and without ions considered.

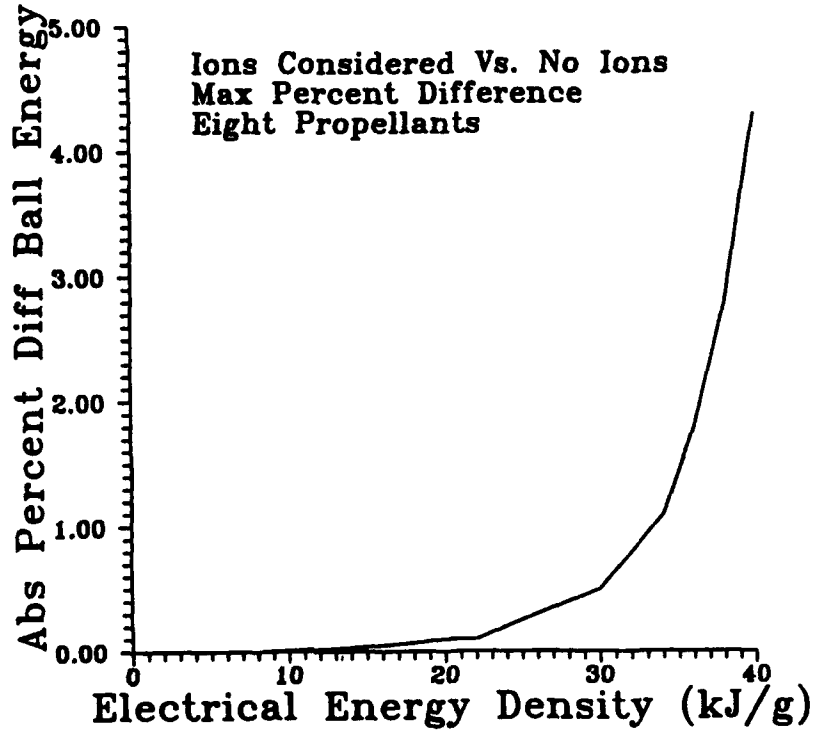

Figure 4. Maximum percent difference in ballistic energy for all eight propellant systems investigated.

inclusion of ions in the thermodynamic calculations is unimportant. Therefore, the program of choice to modify for ETC propellants is BLAKE with a suitably prepared library valid over the range 3,000–10,000 K (or higher).

The contents of the new library (which will be called the extended library here, in distinction to the standard library) were limited by the following two constraints: BLAKE cannot deal with more than 29 gaseous species in any one run, and there were no data for compounds of potassium or magnesium (the two elements most commonly occurring in inorganic additives) in McBride's files. Therefore, the new library was limited to 31 gases, and no condensed phases were included. These 31 gases comprise 29 species containing C, H, N, or O, or combinations of them, plus helium and argon. The limit of 29 gases means that, in the few cases in which either helium or argon is included in the chamber, a REJect instruction would be needed. To avoid this requirement (which is unpopular with some users), the CONstituent instructions for the species O_3 and $H_2C{=}C$ have been displaced by six columns (resulting in their omission), but their STR instructions have been left intact. These species are almost never significant in ETC computations. If a need for either of them should arise, it is a simple matter to restore them.

4. NBLAKE AND ITS LIBRARY

The revised program has been temporarily named NBLAKE to make it easier for testers to keep both the old and new programs in their computers. When testing is completed, the name will revert to BLAKE, version 218.0.

The only major change to the program concerns the way it handles the library. The primary concern was to attempt to minimize the chance of using the standard library in place of the extended library and vice versa. The selection of the library is made by the user prior to running the program, either by explicitly copying the appropriate library from storage to the library file, or (preferably) by choosing one of two batch files (each specific to a particular library) that accomplishes the same result. The only way that users will be aware that they have made the wrong choice will be if they attempt to use the extended library on a formulation containing elements other than C, H, O, or N (the program will immediately abort). It seemed desirable, at the least, to print information identifying the library that was used. This information is now stored in the first line of the alphanumeric file of each library. As a result, the new library cannot be used with any preceding version of BLAKE, and older versions of the library will not work with the new program.

A few revisions were made in the standard library as follows: the data for the condensed phases of K_2S, K_2CO_3, and K_2SO_4 were revised; the species HNO, $AlCl_2$, and $AlCl_3$ were added; and the species C_2H and C_2N were removed.

Some lesser changes were made to the program as follows. (1) The output from the COMposition instruction has been reformatted to fit into 80 columns. (2) Many, but not all, of the messages printed by the program have been changed from all UPPER CASE to the conventional mixture of Upper and Lower Case. (3) The DATe instruction is no longer active. The program will ignore it if used but will not issue an error message. (4) The CMT (CoMmenT) instruction has been deleted. The program will ignore it if used but will not issue an error message. (5) The FORmula instruction has been changed to permit a formula name to be redefined in the same run. (6) The default of the ECHo instruction has been changed from "off" to "on." Also, the appearance of the echoed instructions has been changed. (7) The program can now optionally read a file containing ingredient data. (8) Some changes have been made in the list of prestored ingredients; some other changes had been made prior to the present work. (9) The FORmula instruction was modified to permit the optional entry of energies in joules/mole instead of the default kilocalories/mole. (10) The GUN instruction was modified to permit the direct entry of electrical energy into the system.

Further details on all of these changes will be found in the program documentation being prepared.

5. TEST CASES AND RESULTS

Once the program was modified, two important questions remained: (1) Did the extended temperature library produce equivalent results with the standard library for overlapping temperature ranges (3,000–5,000 K)? and (2) To what extent do the calculated thermochemical values change in using the extended temperature library vs. the standard library? To address these questions, calculations were performed using the two thermochemical data libraries with varying electrical energy densities (equivalent to varying the temperature) for five propellant systems. Three of the systems, pseudo-M30, WC890, and Decalin/70% H_2O_2, were exothermic, while the other two, methanol and water, were endothermic. Results for three of the propellant systems will be presented in this paper to illustrate the effects of calculations using the different libraries.

The percent difference in ballistic energy is computed using the following formula:

$$\% \text{ Diff.} = \frac{\text{B.E. (Standard Lib)} - \text{B.E. (Extended Lib)}}{\text{B.E. (Standard Lib)}} * 100 . \quad (6)$$

Temperature and ballistic energy results at selected electrical energy densities for pseudo-M30 are presented in Table 2 with the percent difference in ballistic energy shown in Figure 5.

Table 2 and Figure 5 show that for pseudo-M30 in the overlapping temperature range (3,000–5,000 K) the differences in computed temperatures and ballistic energies are less than 1%. Both the standard and extended BLAKE libraries use the same fitting formula. The standard library is essentially the one that has been used with BLAKE for years; it was based on JANAF data that were current at the time. The extended library, on the other hand, is new; it is based on McBride's independent results. Considering the difference in the sources of the data for the two libraries, we feel that the computed thermodynamic properties are virtually the same in the overlapping temperature ranges. Thus, the libraries produce equivalent results, as one would hope, in the overlapping temperature range. The percent differences in ballistic energies above 5,000 K, where the libraries do not have overlapping ranges, are not significantly larger in magnitude for temperatures up to 10,000 K (2.4% absolute maximum) but increase in magnitude to exceed +6% as the temperature increases. Therefore, for pseudo-M30, the use of the extended temperature library does not appear to have a significant impact on calculated thermochemical values until gas temperatures exceed 10,000 K. However, these types of results are very dependent on the propellant system, as illustrated by the final two propellant systems discussed in this paper.

Results from similar calculations for Decalin plus 70% hydrogen peroxide are given in Table 3 and Figure 6. As can be seen from the table and figure, the differences in the computed values are quite significant outside of the overlapping temperature range (below 3,000 K and above 5,000 K) with percent differences in ballistic energy up to 25% (less than 2% in the overlapping temperature range). Temperature differences are not as severe as for ballistic energy. This propellant system illustrates the potential errors which can arise when thermochemical data are extrapolated.

Both previous propellant systems discussed were for exothermic propellants. To determine the effect of using the different libraries for an endothermic propellant system, the final system discussed will be methanol. Results are provided in Table 4 and Figure 7. The differences in this case are even more

Table 2. Computed Temperature and Ballistic Energy Results for Pseudo-M30 Using the Standard and Extended Temperature Libraries

Electrical Energy Density (kJ/)	Temperature (K)		Ballistic Energy (J/g)		Diff. B.E. (%)
	Stand.	Extend.	Stand.	Extend.	
0.00	3,036	3,024	4,493	4,509	-0.36
1.00	3,634	3,619	5,562	5,588	-0.47
5.00	5,350	5,347	8,630	8,737	-1.24
10.00	6,914	6,933	11,518	11,570	-0.45
15.00	8,403	8,464	14,502	14,474	0.19
20.00	9,837	9,943	17,529	17,947	-2.38
25.00	11,191	11,314	20,470	21,737	-6.19

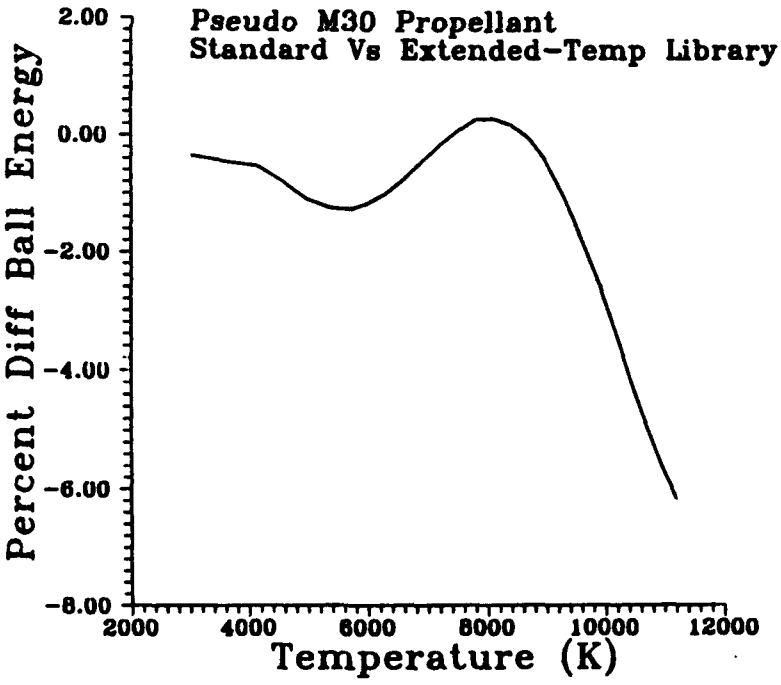

Figure 5. Percent difference in computed ballistic energy using the extended temperature and standard libraries for pseudo-M30.

Table 3. Computed Temperature and Ballistic Energy Results for Decalin Plus 70% Hydrogen Peroxide Using the Standard and Extended Temperature Libraries

Electrical Energy Density (kJ/g)	Temperature (K)		Ballistic Energy (J/g)		Diff. B.E. (%)
	Stand.	Extend.	Stand.	Extend.	
5.50	2,465	2,410	6,247	5,094	18.46
6.00	2,601	2,556	6,660	5,938	10.84
7.00	2,875	2,839	7,489	7,211	3.71
8.00	3,152	3,119	8,322	8,195	1.53
9.00	3,436	3,406	9,180	9,085	1.03
10.00	3,727	3,700	10,071	9,973	0.97
15.00	5,156	5,118	14,698	14,514	1.25
20.00	6,404	6,312	19,191	18,300	4.64
25.00	7,509	7,367	23,732	21,392	9.86
30.00	8,511	8,345	28,494	24,153	15.23
35.00	9,431	9,268	33,571	26,778	20.23
40.00	10,283	10,156	39,126	29,315	25.08

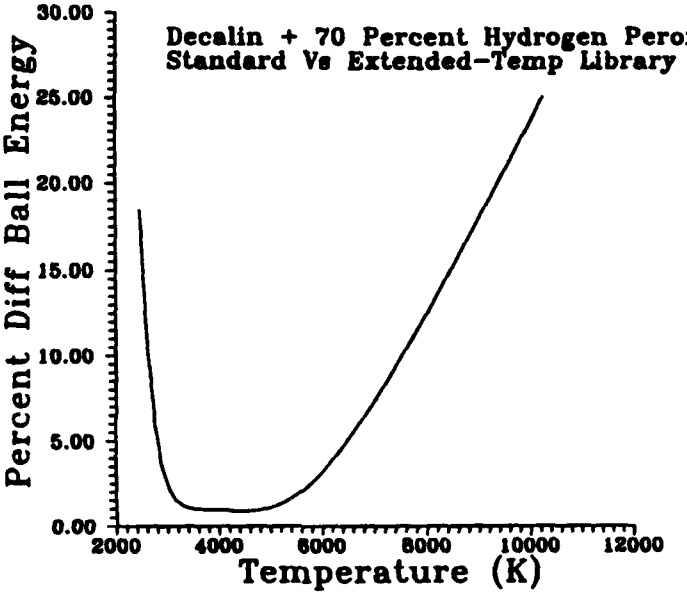

Figure 6. Percent difference in computed ballistic energy using the extended temperature and standard libraries for Decalin plus 70% hydrogen peroxide.

Table 4. Computed Temperature and Ballistic Energy Results for Methanol Using the Standard and Extended Temperature Libraries

Electrical Energy Density (kJ/g)	Temperature (K)		Ballistic Energy (J/g)		Diff. B.E. (%)
	Stand.	Extend.	Stand.	Extend.	
8.00	2,619	2,576	7,264	6,564	9.64
9.00	2,880	2,846	8,123	7,845	3.42
10.00	3,154	3,125	9,032	8,916	1.28
15.00	4,544	4,528	13,864	13,800	0.46
20.00	5,768	5,743	18,541	18,252	1.56
25.00	6,835	6,790	123,165	21,852	5.67
30.00	7,799	7,739	28,048	24,880	11.29
35.00	8,688	8,627	33,380	27,593	17.34
40.00	9,515	9,475	39,300	30,129	23.34
45.00	10,359	10,384	46,715	32,765	34.09
50.00	10,999	11,126	53,803	34,788	35.34

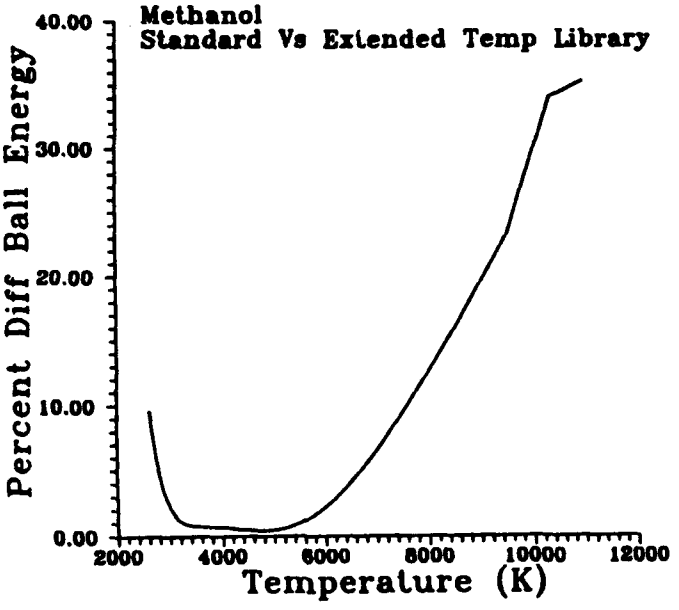

Figure 7. Percent difference in computed ballistic energy using the extended temperature and standard libraries for methanol.

pronounced than in the previous two cases. Such differences are apparently more pronounced with carbon-deficient systems. The reason for this may be explored at a later date.

6. SUMMARY

Results presented in this paper have shown that the formation of ions can be safely ignored in thermodynamic computations for ballistic applications at temperatures up to at least 10,000 K. Using data from NASA's Lewis Research Center, a new library for BLAKE for use at temperatures between 3,000 K and at least 10,000 K has been created. Some minor modifications have been made in the program to facilitate its use with ETC systems. Comparison of results below 3,000 K and above 5,000 K show some significant differences in computed thermochemical data between the two libraries, especially with carbon-deficient propellant systems.

7. REFERENCES

Chase, M. W. Private communication. Dow Chemical Company, Midland, MI (now at the National Institute for Standards and Technology), 1985.

Chase, M. W., C. A. Davies, J. R. Downey, D. J. Frurip, R. A. McDonald, and A. N. Syverud. "JANAF Thermochemical Tables," 3rd ed., American Chemical Society/American Institute of Physics (ACS/AIP), Washington D.C., 1986; also in Journal of Physical and Chemical Reference Data, vol. 14, supplement No. 1, 1986.

Cowperthwaite, M., and W. H. Zwisler. "Tiger Computer Program Documentation." Z106, Standford Research International, Menlo Park, CA, 1973.

Freedman, E. "BLAKE—A Thermodynamics Code Based on TIGER: User's Guide and Manual." ARBRL-TR-02411, U.S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, July 1982.

Gordon, S., and B. J. McBride. "Computer Program for Computation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock, and Chapman-Jouguet Detonation." NASA SP-273, National Aeronautics and Space Administration, Cleveland, OH, 1971.

Kotlar, A. J. Private communication. U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, 1991.

McBride, B. J. Private communication. NASA Lewis Research Center, private communication, 1992.

Svehla, R. A., and B. J. McBride. "Fortran IV Computer Program for Calculation of Thermodynamic and Transport Properties of Complex Chemical Systems." NASA TD 7056, National Aeronautics and Space Administration, Cleveland, OH, 1973.

Volk, F., and H. Bathelt. "Rechnenprogramm zuer Ermittelung del Leistungsdaten von Treibladenspulvern und Raketentreibstoffen undter Verwendung der Virialgleichung." Institute for Chemistry of Propellants (ICT) Report, Pfinztal-Berghausen, Germany, May 1978; Propellants and Explosives, vol. 1, p. 7, 1976.

Wren, G. P., and W. F. Oberle. "A Coupled Thermochemistry-Interior Ballistic Model and Applications to Electrothermal-Chemical (ETC) Guns." ARL-TR-63, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD, February 1993.

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APPENDIX:

PREPARATION OF A THERMODYNAMICS PROGRAM AND LIBRARY FOR USE WITH ETC SYSTEMS

Aside from minor format changes, this appendix is presented in its original form without editorial changes or comments.

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Report EFA-00005-PGA

16 February 1994
Revision 2

PREPARATION OF A THERMODYNAMICS PROGRAM AND LIBRARY FOR USE WITH ETC SYSTEMS

Final Report on

Contract DAAA15-92-D-0001

Task Order Number 3

Prepared for

Paul Gough Associates, Inc.

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FINAL REPORT

Preparation of a Thermodynamics Program and Library for Use With ETC Systems

Reference: Contract DAAA15-92-D-0001
Task Order Number 3

Work Performed by: Eli Freedman & Associates

Period Covered: 10 June–31 December 1992

ABSTRACT

The goal of this task was to produce a thermodynamics program and its accompanying library for use with electrothermal-combustion propellant (ETC) systems at temperatures up to 10,000 K. It was first necessary to decide whether ions had to be taken into account in such a program. For this purpose, a new program called EXMuCET was produced. It is a modification for use at temperatures above 6,000 K of an earlier program called MuCET, a microcomputer version of the NASA-Lewis thermochemistry program CET86. This program was applied to 9 different propellant mixes; the results showed that the formation of ions could be safely neglected at temperatures up to 10,000 K at the gas densities to be expected in ETC formulations. This meant that 'Blake' would be the program used.

A 'Blake' library for the temperature range 4,000 K–10,000 K was created and tested. The testing consisted of comparing results from the new library with those obtained using the accepted standard library in the overlap temperature range, 4,000 K–5,000 K. The results of the testing depend to a small extent on whether the REJect instructions are used. Overall the differences in impetus between the two sets of results are less than 0.3%.

ACKNOWLEDGMENTS

It is a pleasure to thank Ms. Bonnie McBride, National Aeronautics and Space Administration, Lewis Research Center, Cleveland, Ohio, for her invaluable assistance. This task could not have been completed without the tables of thermodynamic data and coefficients that she made available to the U.S. Army Research Laboratory.

Also, I want to thank Dr. Anthony J. Kotlar, Mr. William F. Oberle, and Dr. Kevin J. White, all of the U.S. Army Research Laboratory, for helpful comments and advice.

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I. INTRODUCTION

A. *Background.*

1. An electrothermal-combustion (ETC) gun derives part (but not usually all) of its energy from a high-power electrical discharge. One of the consequences of this discharge is that initially the chamber temperatures are very high (10,000–20,000 K), which may cause ionization.

2. The computation of the performance of any gun requires for its input thermodynamic data about its propellant. The 'Blake' code is one of the most widely used programs for such calculations, but it has drawbacks for application to ETC problems:

a. The heat capacities of the products in its library are fitted as a function of temperature only up to 5,000 K.

b. The empirical formula that it uses for fitting is not well-suited for covering the entire temperature range from, say, 500 K to 10,000 K.

c. This code cannot deal with systems containing ions.

B. *Goals.* The objective of this task was to provide a unified thermodynamics code that can produce all of the customary thermochemical data for candidate electrothermal propellants. This code is to have the following features:

1. It will be a unified thermodynamics code that produces all of the customary thermochemical data for candidate electrothermal propellants.

2. It will cover the temperature range from 1,000 K to 10,000 K or higher.

3. It will furnish the frozen gamma of the equilibrium composition.

4. It will estimate the covolume of the equilibrium system.

II. APPROACH

A. *Possible Codes.* There are essentially only two choices for the code, either 'Blake' or the NASA-Lewis code, CET89 (or variants of it or of its predecessor, CET86).

1. CET89 is an outstanding program with major advantages and major disadvantages.

a. It can easily work with ions.

b. BUT: It works only for ideal gases, and therefore cannot estimate covolumes. If it were to be adopted, a modification or a separate program would have to be developed to supply this deficiency.

2. In most respects 'Blake' does not run as easily as CET89, but it was designed for use primarily with non-ideal gases and the propellant covolume is one of its primary outputs. If it can be shown that the formation of ions is not of importance at temperatures up to 10,000 K, then 'Blake' will be chosen.

There will remain the lesser task of providing an extended temperature-range library for use with the program.

B. *Subtasks.* The task was broken down into the following subtasks:

1. Search for thermodynamic data at temperatures up to 10,000 K for significant species.

2. Devise a way of deciding the extent to which ions are formed at temperatures below 15,000 K.

3. Based on the these results, choose either CET89 or 'Blake'.

   a. If ions are significant, then choose CET89 and devise a means of estimating covolumes.

   b. If ions are not significant, then choose 'Blake' and fit the thermodynamic data accordingly.

C. *Thermodynamic Data.* The quest for thermodynamic data was ended even before it started.

1. Bonnie McBride, National Aeronautics and Space Administration, Lewis Research Center (NASA LRC), Cleveland, Ohio, kindly furnished to the U.S. Army Research Laboratory (ARL) a set of coefficients that permit computations up to 15,000 K (and 20,000 K in some cases) for about a hundred species.

2. The format of these tables was different from that used in all of the NASA thermodynamic programs. Hence it was necessary to modify one of them to accept the new format. MuCET, a modification of CET86 for microcomputers, was selected for this purpose. The new program was named EXMuCET.

III. PREPARING EXMuCET

A. *Description of the Formats.*

1. In all of the NASA-Lewis thermochemistry programs through CET89, the heat capacity, Cp, enthalpy, H, and entropy, S, were represented by the empirical formulas

$$Cp/R = a + b*T + c*T^2 + d*T^3 + e*T^4 \quad \{1\}$$

$$H/R*T = a + b*T/2 + c*T^2/3 + d*T^3/4 + e*T^4/5 + f/T \quad \{2\}$$

$$S/R = a*\ln(T) + b*T + c*T^2/2 + d*T^3/3 + e*T^4/4 + g \quad \{3\}$$

R is the gas constant, so Cp/R and S/R are dimensionless; likewise, H/R*T is dimensionless. It should be noted that Cp, H, and S are functionally related:

$$H = \int Cp\,dT + \text{constant; and} \quad \{4\}$$

$$S = \int [Cp/T]\,dT + \text{constant.} \quad \{5\}$$

The integration constants in Eqns. {4} and {5} are denoted by f and g in Eqns. {2} and {3}.

2. The fitting range is split from 300 to 1,000, and 1,000 to 5,000; the values of the three functions are forced to match at the boundary (1,000 K). This makes for 2 sets of a, b, . . . , g. (For ballistic applications, it might be more useful to make the fitting ranges 1,000–2,500, 2,500–6,000, but this point will now be pursued at this time.)

3. In theory this same format could be used for higher temperatures (meaning up to at least 10,000 K, and perhaps up to 20,000 K). Instead, McBride improved the accuracy by splitting the fitting range into 3 parts, with boundaries of 1,000 and 6,000. This format will be called here the "intermediate format."

4. Later, she adopted a different format, called here the "new format":

$$Cp/R = a/T^2 + b/T^1 + c + d*T + e*T^2 + f*T^3 + g*T^4 \quad (6)$$

$$H/R*T = -a/T^2 + (b/T)*\ln(T) + c + d*T/2 + e*T^2/3 + f*T^3/4 + g*T^4/5 + h/T \quad (7)$$

$$S/R = -a/(2*T^2) - b/T + c*\ln(T) + d*T + e*T^2/2 + f*T^3/3 + g*T^4/4 + i \quad (8)$$

H and S are related to Cp just as they were before. The constants a, b, . . . , g are of course different from a, b, . . . , g in Eqns. (1)–(3); h and i are integration constants. Throughout this report, it is this format (Eqns. (6)–(8)) that will be referred to as the "new" format.

5. For the record it should be noted that McBride included provision for an 8th term (j*T^5) in Eqn. (6) with corresponding terms in (7) and (8). To date this term has not been used.

B. *Details of the Changes.*

1. Examination of CET86 showed that only 3 subroutines had to be modified: UTHERM, SEARCH, and CPHS. Technically, Subroutine HCALC should also have been modified, but it was decided not to do so. This subroutine serves to compute the enthalpy of formation of some (not all) input species. This feature is somewhat useful, but its function is largely superseded by Program PREP, which was produced last year by EF&A. (See the documentation of PREP for further details.)

2. The programming was complicated by the need to allow for the future addition of the term j*T^5 in Cp.

3. In addition, two potential difficulties were uncovered.

a. The ranges of the original format were usually 298.15 (or 300) K to 1,000, and 1,000 to 5,000 (or 6,000) K, at least for gases. For liquids, either there was only one range, 300 K to boiling point, or else the two ranges were 300 to 1,000, 1,000 to boiling point, depending on whether the boiling point was below or above 1,000 K. The case with solids was similar, either 300–melting point, or 300–1,000, 1,000–melting point. In all cases, however, the actual ranges were part of the input for each species and thus were available to the program throughout its execution. Therefore, when computations were being run at temperature Tx, the program could decide if Tx was above or below the melting (boiling) point of a solid (liquid), and take appropriate action.

b. In the new format, the ranges are fixed: 300–1,000, 1,000–6,000, and 6,000–10,000. (Note that all three ranges are not necessarily used for every species; the actual number of ranges used is part of the input.) No provision has been made for inputting melting or boiling points. In theory this is not necessary, because only the phase with the most negative free energy can form. In practice, however, owing to artifacts of the fitting process, it is possible for the program to find thermodynamically-impossible phases. This problem has been side-stepped.

c. The second difficulty was similar in some ways. The upper ends of the fitting ranges are not the same; while some of them are 20,000 K, most of them are only 5,000 or 6,000 K. The actual value depends on the available thermochemical data, which in turn reflect physical realities.

d. The new program originally included a test that ensured that the thermochemical functions for a given species were not evaluated outside the species' fitting range. The reason for including this test was indisputable: Owing to the unknown behavior of the fitted thermodynamic functions outside their range of validity, it is possible for the computation to come up with a species under conditions where it is thermodynamically impossible for it to exist. Eventually it was discovered that, in the course of converging, the program occasionally produced intermediate temperatures that were outside the fitting ranges of some species. (NASA's CET86 exhibits similar behavior.) The range check was deleted and the program worked well.

C. *Initial Testing Using a Modified "Old" Library.*

1. Testing was accomplished by comparing results of EXMuCET, the new program, with those from MuCET, a version of CET86 produced by EF&A specifically for use with microcomputers. It was essential that this testing procedure compare only programs, not thermodynamic libraries. For this purpose, 2 additional programs were written.

a. Program OLDINT converted the standard library furnished by NASA's Lewis Research Center for use with CET86 to the intermediate format described in III A 3 above.

b. Program INTNEW converted the library in the intermediate format to the new format. Note that these conversions were accomplished strictly by reformatting the libraries, and adding zeros for the coefficients of powers of T that were not present in the original format. No refitting was done by either program.

c. These two programs were themselves tested by inspection of the results. As an example of this transformation, here are the entries for CH3:

Original Format:

```
CH3               J 6/69C  1.H  3.0  0.0   0.G     300.000  5000.000       15.03470R  1
 0.28400327E 01  0.60869086E-02-0.21740338E-05  0.36042576E-09-0.22725300E-13     2
 0.16449813E 05  0.55056751E 01  0.34666350E 01  0.38301845E-02  0.10116802E-05     3
-0.18859236E-08  0.66803182E-12  0.16313104E 05  0.24172192E 01       0.00000000    4
```

New Format:

```
CH3
2 J 6/69 C  1.00H   3.000   .000   .00    .00        0    15.03470   .00000000E+00
  298.150 1000.000 7 -2.0 -1.0      .0 1.0 2.0      3.0 4.0  .0      .00000000D+00
  .00000000D+00  .34666350D+01  .38301845D-02  .10116802D-05 -.18859236D-08
  .66803182D-12  .00000000D+00  .16313104D+05  .24172192D+01
  1000.000 5000.000 7 -2.0 -1.0     .0 1.0 2.0      3.0 4.0  .0
  .00000000D+00  .00000000D+00  .28400327D+01  .60869086D-02 -.21740338D-05
  .36042576D-09 -.22725300D-13  .00000000D+00  .16449813D+05  .55056751D+01
```

The placement of the high temperature data before the low temperature ones in the original format was one of the little details that complicated an otherwise straightforward programming chore.

d. Using these new programs, the standard NASA library, FILE4.DAT, was transformed to the new format; the resulting library was named NEWFILE.DAT. A number of test cases were run with MuCET and EXMuCET using FILE4.DAT or NEWFILE.DAT, as appropriate.

e. Overall the comparison was excellent, but a problem caused by the occurrence (or non-occurrence) of condensed phases was revealed. The magnitude of this problem in a typical case can be seen by comparing the output from 3 runs.

Run A: MuCET with FILE4.DAT, no species omitted.
Run B: MuCET with FILE4.DAT, all condensed species omitted.
Run C: EXMuCET with NEWFILE.DAT.

RUN:	A	B	C
THERMODYNAMIC PROPERTIES			
P, MPA	214.56	214.49	214.49
T, DEG K	2999.8	2998.8	2998.8
RHO, KG/CU M	200.0	200.0	200.00
H, KJ/KG	-508.57	-508.88	-508.88
U, KJ/KG	-1581.35	-1581.35	-1581.35
S, KJ/(KG)(K)	9.4105	9.4104	9.4104
CP, KJ/(KG)(K)	1.9638	1.9644	1.9644
CP FROZN, J/G-K	1.8672	1.8668	1.8668
EQUILIB GAMMA	1.2275	1.2275	1.2275
FROZEN GAMMA	1.2369	1.2370	1.2370
IMPETUS, J/G	1072.8	1072.5	1072.5
BALLERGY*, J/G	4528.5	4525.6	4525.6

* Ballergy = Impetus/(gamma - 1)

A more sensitive comparison is furnished by the comparison of the computed mole fractions:

Run	A		B		C
N2	0.27696	N2	0.27698	N2	0.27698
CO	0.27467	CO	0.27469	CO	0.27469
H2O	0.24156	H2O	0.24163	H2O	0.24163
H2	0.13166	H2	0.13173	H2	0.13173
CO2	0.06932	CO2	0.06933	CO2	0.06933
HF	0.00179	HF	0.00149	HF	0.00149
H	0.00124	H	0.00123	H	0.00123
OH	0.00077	OH	0.00077	OH	0.00077
NAOH	0.00076	NAOH	0.00077	NAOH	0.00077
NH3	0.00038	NH3	0.00038	NH3	0.00038
NA	0.00016	ALF2O	0.00023	ALF2O	0.00023
AL2O3(L)	0.00011	NA	0.00017	NA	0.00017
NO	0.00011	NO	0.00011	NO	0.00011
HCN	0.00011	HCN	0.00011	HCN	0.00011
ALF2O	0.00008	ALO2H	0.00007	ALO2H	0.00007
HCO RAD	0.00006	HCO RAD	0.00006	HCO RAD	0.00006
(HCOOH)2	0.00005	(HCOOH)2	0.00005	(HCOOH)2	0.00005
HCHO	0.00004	HCHO	0.00004	HCHO	0.00004
NAH	0.00003	NAH	0.00003	NAH	0.00003
NAF	0.00003	NAF	0.00003	NAF	0.00003
HNCO	0.00003	HNCO	0.00003	HNCO	0.00003
ALO2H	0.00002	NACN	0.00001	NACN	0.00001
NACN	0.00001	NH2	0.00001	NH2	0.00001
NH2	0.00001	CH4	0.00001	CH4	0.00001
CH4	0.00001	ALOH	0.00001	ALOH	0.00001
		ALOF	0.00001	ALOF	0.00001

f. Evidently the effect is real but quite small. Since ETC propellants do not form any condensed phases at chamber conditions, the problem is not serious.

g. Another way of looking at this same problem is to consider the effect of adding electrical energy to a propellant mix that forms graphite (solid carbon) in the absence of added energy. Such a composition is a stoichiometric mixture of decalin with 70% hydrogen peroxide.

Using FILE4.DAT, MuCET gives

DECALIN + 70% HYDROGEN PEROXIDE + VARYING ENERGY

CHEMICAL FORMULA	WT FRAC	ENERGY KJ/KG-MOL	S	T (K)
FUEL C 10.000 H 18.000	1.00000	-230538.	L	298.1
OXID H 2.000 O 2.000	.70000	-187778.	L	298.1
OXID H 2.000 O 1.000	.30000	-285830.	L	298.1

THERMODYNAMIC PROPERTIES

Elec Nrgy, J/G	0	1000.	2000.
U, J/G	-5145.85	-4145.85	-3145.85
P, MPA	99.797	123.77	150.32
T, DEG K	1271.7	1431.0	1586.9
CP EQ, J/G-K	7.1134	8.2267	7.9425
CP FROZ, J/G-K	2.7930	2.8810	2.9433
EQUILIB GAMMA	1.1326	1.1427	1.1589
FROZEN GAMMA	1.1634	1.1766	1.1918
IMPETUS, J/G	499.0	618.9	751.6
BALLERGY, J/G	3052.9	3503.7	3919.1

MOLE FRACTIONS

HCHO	0.00002	HCHO	0.00005	HCHO	0.00010
(HCOOH)2	0.00002	(HCOOH)2	0.00002	(HCOOH)2	0.00003
CH4	0.26007	CH4	0.24128	CH3	0.00001
CH3OH	0.00001	CH3OH	0.00001	CH4	0.22032
CO	0.10092	CO	0.19191	CH3OH	0.00002
CO2	0.09098	CO2	0.06541	CO	0.27833
C2H4	0.00004	C2H4	0.00015	CO2	0.04009
ETHANE	0.00052	CH3CHO	0.00001	C2H4	0.00001
H2	0.14913	ETHANE	0.00068	KETENE	0.00001
H2O	0.22097	n-C3H6	0.00001	C2H4	0.00039
C(GR)	0.17731	PROPANE	0.00001	CH3CHO	0.00001
		H2	0.21653	ETHANE	0.00081
		H2O	0.16898	n-C3H6	0.00002
		C(GR)	0.11495	PROPANE	0.00001
		H2	0.28297	H2	0.34901
		H2O	0.11972	H2O	0.07599
		C(GR)	0.05715	C(GR)	0.01526

THERMODYNAMIC PROPERTIES

Elec Nrgy, J/G	3000.	4000.	5000.
U, J/G	-2145.85	-1145.85	-145.85
P, MPA	180.97	217.04	257.55
T, DEG K	1763.2	1978.7	2234.5
CP EQ, J/G-K	6.7622	5.5394	4.7839
CP FROZ, J/G-K	2.9984	3.0536	3.1056
EQUILIB GAMMA	1.1789	1.2074	1.2124
FROZEN GAMMA	1.2065	1.2189	1.2278
IMPETUS, J/G	904.8	1085.2	1287.8
BALLERGY, J/G	4381.9	4957.0	5651.9

MOLE FRACTIONS

HCHO	0.00015	HCHO	0.00022	HCHO	0.00028
(HCOOH)2	0.00002	(HCOOH)2	0.00001	(HCOOH)2	0.00001
CH3	0.00005	CH3	0.00017	CH3	0.00053
CH4	0.19312	CH4	0.15654	CH4	0.12068
CH3OH	0.00002	CH3OH	0.00002	CH3OH	0.00002
CO	0.34392	CO	0.37579	CO	0.38422
CO2	0.02050	CO2	0.00900	CO2	0.00385
C2H4	0.00005	C2H4	0.00030	C2H4	0.00144
KETENE	0.00003	KETENE	0.00007	KETENE	0.00013
C2H4	0.00089	C2H4	0.00177	C2H3 RAD	0.00002
CH3CHO	0.00002	CH3CHO	0.00002	C2H4	0.00313
ETHANE	0.00090	C2H5	0.00001	CH3CHO	0.00003
n-C3H6	0.00004	ETHANE	0.00088	C2H5	0.00004
PROPANE	0.00001	PROPYNE	0.00001	ETHANE	0.00078
ALLENE	0.00001	C3H3 RAD	0.00001		
C3H5 RAD	0.00001	PROPYNE	0.00006		
n-C3H6	0.00009	ALLENE	0.00005		

Using NEWFILE.DAT, EXMUCET gives

DECALIN + 70% HYDROGEN PEROXIDE + VARYING ENERGY

CHEMICAL FORMULA	WT FRAC	ENERGY J/KG-MOL	S	T (K)
FUEL C 10.000 H 18.000	1.00000	-230538.	L	298.1
OXID H 2.000 O 2.000	.70000	187778.	L	298.1
OXID H 2.000 O 1.000	.30000	285830.	L	298.1

THERMODYNAMIC PROPERTIES

ELEC NRGY, J/G	0.0	1000.	2000.
U, J/G	-5145.85	-4145.85	-3145.85
P, MPA	94.913	119.50	147.73
T, DEG K	1220.6	1392.1	1567.4
CP EQ, J/G-K	6.8719	7.3472	7.1432
CP FROZ, J/G-K	2.7409	2.8463	2.9285
EQUILIB GAMMA	1.1364	1.1534	1.1730
FROZEN GAMMA	1.1653	1.1776	1.1918
IMPETUS, J/G	474.6	597.5	738.6
BALLERGY, J/G	2870.8	3364.9	3851.5

MOLE FRACTIONS

HCHO	0.00002	HCHO	0.00005	HCHO	0.00010
(HCOOH)2	0.00002	(HCOOH)2	0.00002	(HCOOH)2	0.00002
CH4	0.43043	CH4	0.34248	CH3	0.00001
CH3OH	0.00001	CH3OH	0.00001	CH4	0.26689
CO	0.18553	CO	0.26984	CH3OH	0.00002
CO2	0.15400	CO2	0.08467	CO	0.32442
C2H4	0.00013	KETENE	0.00001	CO2	0.04286
CH3CHO	0.00001	C2H4	0.00030	C2H2	0.00001
ETHANE	0.00151	CH3CHO	0.00001	KETENE	0.00001
n-C3H6	0.00001	ETHANE	0.00138	C2H4	0.00058
PROPANE	0.00002	n-C3H6	0.00002	CH3CHO	0.00002
H2	0.10379	PROPANE	0.00002	ETHANE	0.00119
H2O	0.12453	H2	0.18055	n-C3H6	0.00003
		H2O	0.12064	PROPANE	0.00001
				H2	0.26417
				H2O	0.09966

THERMODYNAMIC PROPERTIES

ELEC NRGY, J/G	3000.	4000.	5000.
U, J/G	-2145.85	-1145.85	-145.85
P, MPA	180.16	217.04	257.55
T, DEG K	1758.8	1978.7	2234.5
CP EQ, J/G-K	6.4774	5.5394	4.7839
CP FROZ, J/G-K	2.9959	3.0536	3.1056
EQUILIB GAMMA	1.1922	1.2074	1.2124
FROZEN GAMMA	1.2062	1.2189	1.2278
IMPETUS, J/G	900.8	1085.2	1287.8
BALLERGY, J/G	4368.4	4957.0	5651.9

MOLE FRACTIONS

HCHO	0.00016		HCHO	0.00022		HCHO	0.00028
(HCOOH)2	0.00002		(HCOOH)2	0.00001		(HCOOH)2	0.00001
CH3	0.00005		CH3	0.00017		CH3	0.00053
CH4	0.20485		CH4	0.15654		CH4	0.12068
CH3OH	0.00002		CH3OH	0.00002		CH3OH	0.00002
CO	0.35719		CO	0.37579		CO	0.38422
CO2	0.02032		CO2	0.00900		CO2	0.00385
C2H2	0.00006		C2H2	0.00030		C2H2	0.00144
KETENE	0.00003		KETENE	0.00007		KETENE	0.00013
C2H4	0.00101		C2H4	0.00177		C2H3 RAD	0.00002
CH3CHO	0.00002		CH3CHO	0.00002		C2H4	0.00313
ETHANE	0.00101		C2H5	0.00001		CH3CHO	0.00003
n-C3H6	0.00005		ETHANE	0.00088		C2H5	0.00004
PROPANE	0.00001		PROPYNE	0.00001		ETHANE	0.00078
H2	0.34404		ALLENE	0.00001		C3H3 RAD	0.00001
H2O	0.07115		C3H5 RAD	0.00001		PROPYNE	0.00006
			n-C3H6	0.00009		ALLENE	0.00005
			PROPANE	0.00001		C3H5 RAD	0.00003
			H	0.00002		n-C3H6	0.00015
			HCO RAD	0.00001		PROPANE	0.00001
			H2	0.41098		1,3-C4H6	0.00001
			H2O	0.04406		H	0.00009
			HCO RAD	0.00002			
			H2	0.45978			
			H2O	0.02462			

At temperatures of 1,587 K and below, MuCET shows C(gr) in the products; there are moderate differences in the thermodynamic properties computed by the two programs in the same region. This difference decreases at 1,759 K and vanishes at 1,979 K. This point could have been made even stronger by adding energy in increments smaller than 1,000 J/g. Since EXMuCET will be used primarily for temperatures above 5,000 K, this problem with the omission of condensed phases is not important and will be ignored.

D. *Initial Testing Using the Extended "New" Library.*

1. Early tests with EXMuCET using McBride's extended library gave terrible results.

a. The most serious problem was that the new (extended range) library gave flame temperatures around 9,300 K!

b. Furthermore, many of the test cases would not even run with the extended library. The output gave the uninformative message, SINGULAR MATRIX. This was eventually traced to the lack of data for compounds of potassium, sodium, fluorine, aluminum, and magnesium in the new library. These compounds are used as flash suppressants or stabilizers in many propellants. Accordingly all of them were removed from all of the compositions; the new compositions are labelled "pseudo-. . . " to emphasize this change.

2. The previous testing of EXMuCET using the transformed standard library had given no indications of trouble (see Section C, above). Based on those results, we looked elsewhere for the problem. The first hypothesis was that there was a problem with the database. In view of the well-deserved high reputation of NASA's Lewis Research Center, this hypothesis seemed very unlikely, but it could not be ruled out *a priori*. As will be seen below, this hypothesis was false.

3. Testing the data base required writing a new program, CALCTH.FOR, whose purpose was to generate tables of the thermodynamic functions. The results for N atoms were obviously incorrect. This problem was readily corrected. It turned out that there was a similar problem in Subroutine EXUTHERM in EXMuCET, which was also corrected.

E. *Testing EXMuCET with Different Libraries.* It was shown above that EXMuCET gives the same results with McBride's standard library transformed to the new format as MuCET does with the standard untransformed library. The more interesting question remained, Would EXMuCET give the same results at temperatures below 5,000 K with the extended library as MuCET does with the standard library?

1. To this end, a DOS batch file, TESTLIBS.BAT, was written (see listing in Appendix A). This file first creates two binary libraries for use with EXMuCET. The first library was taken from the NASA library distributed with CET89 (suitably transformed for use with EXMuCET—see above for details). The second library was McBride's extended library. The two binary libraries were saved for later use. The same test cases were run with each library and the results compared.

2. It was deemed necessary not only to run a number of different test cases, but also to run each of them with a series of added electrical energies so as to be sure of covering the temperature range up to 5,000 K and even a little beyond. Generating the input for such tests was too tedious to be undertaken

by hand, so a QuickBasic program, MAKEINP.BAS, was written that automated most of the work. It is listed in Appendix B.

a. The user inputs the desired starting energy, the energy increment, and the final energy (all in Joules/g). The program reads a template containing the input for 8 propellants, including the NAMELIST, and then produces a properly-formatted input file for EXMuCET for all the compositions at each energy; next, it produces a second, almost-identical file, except that in this case, the NAMELIST contains the option, IONS=T.

b. The eight propellants or propellant systems used were:

1. Pseudo M30
2. Pseudo WC890
3. JA-2
4. M9
5. M1
6. Decalin + WFNA*
7. Decalin + 70% H_2O_2
8. RFNA* + UDMH*

* RFNA = red fuming nitric acid. UDMH = unsymmetrical dimethyl hydrazine. WFNA = white fuming nitric acid.

Details of these compositions are given in Appendix C, where the template is printed.

c. The title of each case lists the added energy as "# Joules/g"; the program changes the "#" to amount of added electricity chosen by the user. The NAMELIST contains the option, "U=#"; here, the program properly changes the "#" to the correct total energy of the system, which includes both the initial energy of the composition as well as the added electrical energy. For simplicity all of the energies are in Joules.

3. The SUMMARY files for different outputs produced by EXMuCET are then compared by a QuickBasic program, COMPARE.BAS, which is listed in Appendix D.

The various files differ from each other according to which thermodynamics library was used to produce them, and whether or not ions were permitted to form.

a. COMPARE identifies the thermodynamics libraries being used and the names of the input files, which are printed for positive identification of the output.

b. It then proceeds to compare temperatures, impetus, gammas, and ballistic energies (labelled "ballergy" in the output) for any two specified files; it also computes various measures of agreement.

c. The results obtained after the final corrections to the program were better overall, but still showed problems, at least at the lower temperatures. Examination of the file OUTPUT revealed the occurrence of the message "ADD H2O (L)" even though the approximate flame temperature was 3,200 K! The upper range for the thermodynamics data for H_2O (liq) in the library is 400–600 K; owing to an apparent defect in the programming, this fact is not being used by the program to eliminate H_2O (liq) from consideration. This defect remains elusive in spite of additional effort. Pending its removal, all condensed phases (including graphite) have been eliminated from the database. This is admittedly inelegant; on the other hand, EXMuCET is intended for use at temperatures above 5,000 K, where no condensed phases exist.

4. The final results of the various comparisons are given in Appendixes E, F, and G. The nomenclature for the various files is as follows. The root of all names is TSTLB. To this is appended in order

S or O for SUMMARY or OUTPUT, respectively, and
NO or IO for NO [ions] or IO [ions included], respectively.

5. There are only small differences in the results produced using the standard (CET89) library compared to those produced using the extended library.

a. Further evidence that the two libraries are in virtually complete agreement with each other is shown by a comparison of the amounts of products produced by each. Appendix H gives such a comparison for one case, composition 1 (pseudo M30) at loading density = 0.2 g/cc and with 5,000 J/g of added energy. This is an extremely sensitive test, so the agreement is quite satisfying.

b. Most important of all, the results show conclusively that regardless of which thermodynamics library is used, the omission or inclusion of ions has no effect. Therefore the program of choice for use with ETC propellants is 'Blake' with a suitably prepared library.

F. *Intercomparison of Various Thermodynamic Tables and Coefficients.*

1. The principal database on which the present work is based is the set of coefficients for approximately 133 C-H-O-N species obtained from McBride (NASA LRC). The value of this set to the present work cannot be overestimated; nothing could have been done without it. Nevertheless, when tables of thermodynamic data for 28 C-H-O-N species were belatedly sent to ARL by the National Standard Data Reference System of the National Institute for Standards and Technology (NIST) (formerly the National Bureau of Standards), it appeared prudent to compare them with tables produced using the LRC coefficients. These species are listed in Appendix I.

To this end two new programs were written.

a. XCALCTH4 is a variant of the program CALCTH previously mentioned in Sect. III.D.3 above.

i. The input to XCALCTH4 was an edited subset of the LRC coefficients. This editing reduced it to the 28 species in the NIST tables and converted their names so that they were identical in both sets. This was necessary to ensure that identical species were being compared.

ii. The output from XCALCTH4 was a table of the temperature, T, and the three principal thermodynamic functions: the heat capacity, $C_p(T)$; the entropy, S(T); and the enthalpy of formation at 298 K plus the increment in enthalpy from 298 K to T, Delta $H_f(298) + H(t) - H(298)$. Each of these entries was set off by commas to make them suitable for input to the next program, COMPARE3.

b. COMPARE3 is a BASIC program that compares the two sets of tables at every temperature for each species. It was programmed to take into account the fact that the increments in temperatures in the two tables might be different (in which case only the values at the larger increments were used); and the fact that one table might end before the other. This was because some of the species in the LRC set were fitted only to 6,000 K, while the NIST tables went uniformly to 10,000 K.

c. The results of the comparison are given in Appendix J, which gives the mean absolute deviation and the root-mean-square percent deviations for the three principal thermodynamic functions. The table has been sorted in order of increasing RMS percentage error in the enthalpy.

i. Overall the comparison is satisfactory: Only three species have RMS errors in their enthalpies exceeding 5%, and they are all ions, which will be of little or no importance in determining the range of validity of EXMuCET.

ii. There is no way of deciding from this comparison alone which set of data is the better. The important point is that they are consistent.

IV. ESTABLISHING THE NEW LIBRARY

A. The next step was the determination of the 29 species that would constitute the new 'Blake' library. This limit is imposed by the program itself; it could be raised to about 35 without too much extra work, but there does not appear to be any compelling reason for this change.

1. To this end, 8 propellant systems, listed in Table 1, were selected.

Table 1. Systems Studied for Determining Important Species

1. Pseudo M30	5. M1
2. Pseudo WC890	6. Decalin + WFNA
3. JA-2	7. Decalin + 70% H_2O_2
4. M9	8. RFNA + UDMH

These systems were then evaluated with EXMuCET for a wide range of added energies (from 0 to as much as 40,000 J/g); the highest resulting temperature was 12,924 K. The output from these calculations was then sorted in order of decreasing mole fraction for each species, and then all entries with mole fractions less than 1×10^{-3} were deleted. The results are shown in Table 2.

The column labelled "Maximum" is self-explanatory. The column labelled "Minimum" lists, for a given species, the smallest computed mole fraction greater than 1×10^{-3} for that species, and the corresponding temperature.

Table 2. Concentrations of Various Species Produced in Nine Different Propellant Systems with Varying Added Energies

		MAXIMUM		MINIMUM*	
	Name	Mole Frac	Temp (K)	Mole Frac	Temp (K)
1.	H_2	0.5485	3675.	0.0173	12924.
2.	CO	0.5062	2491.	0.0764	11793.
3.	CH_4	0.4312	1217.	0.0014	8017.
4.	H_2O	0.4278	3739.	0.0022	12924.
5.	H	0.3543	11793.	0.0011	2950.
6.	O	0.2857	12924.	0.0010	3812.
7.	N_2	0.2774	3010.	0.0129	12398.
8.	CO_2	0.2068	3812.	0.0010	8017.
9.	OH	0.1446	6281.	0.0031	6145.
10.	N	0.0926	12383.	0.0017	6281.
11.	C	0.0801	12416.	0.0011	7990.
12.	NO	0.0519	7517.	0.0016	3575.
13.	O_2	0.0400	6281.	0.0013	5091.
14.	Acetylene	0.0331	5041.	0.0012	2233.
15.	CN	0.0305	12383.	0.0015	8465.
16.	NH	0.0223	11793.	0.0013	6281.
17.	CH	0.0189	8882.	0.0016	8162.
18.	C_2H	0.0182	8882.	0.0010	11424.
19.	HCO	0.0109	8882.	0.0010	5388.
20.	CH_2	0.0104	8882.	0.0011	9532.
21.	CH_3	0.0084	5041.	0.0033	8882.
22.	C_2	0.0064	12416.	0.0012	10977.
23.	NH_2	0.0044	11793.	0.0010	6776.
24.	HCN	0.0037	9532.	0.0010	6599.
25.	Ethylene	0.0034	3675.	0.0010	5041.
26.	CCO (radical)	0.0029	12416.	0.0012	10977.
27.	O_3	0.0023	12924.	0.0013	12647.
28.	HO_2	0.0022	6281.	0.0010	9604.
29.	Vinylidene#	0.0022	6145.	0.0014	8882.
	---------- CUT-OFF for 'Blake' ----------				
	HNO	0.0019	8465.	0.0010	10409.
	[ELECTRONS	0.0018	12924.	0.0010	12035.]
	NCN	0.0018	11456.	0.0012	9280.
	ETHANE	0.0015	1217.	0.0015	1217.
	NH3	0.0014	11793.	0.0011	12454.

* "Minimum" here refers to the smallest mole fraction greater than 1×10^{-3}.
# This is the radical $H_2C{=}C$.

The significance of Table 2 can be made clear by examining some of the early entries in more detail. Hydrogen (H_2) is an important product whose concentration reaches a maximum (0.55) at 3,675 K and then declines to 0.017 at 12,294 K, which is the highest temperature studied. Carbon monoxide (CO) behaves similarly. Methane (CH_4) reaches its maximum concentration at a lower temperature, and then declines until it becomes 0.001 at 8,017 K; its mole fraction at all higher temperatures is less than 0.00100. Water (H_2O) behaves similarly to H_2. Hydrogen atom (H) is different: Its mole fraction is less than 0.00100 at temperatures below 2,950 K; its concentration increases with increasing temperature until it reaches a maximum at 11,793 K. Oxygen atom (O) behaves similarly.

In its present form, 'Blake' is limited to working with 29 gaseous species at any one time. Therefore, based on the results in Table 2, the 29 species that had maximum concentrations equal to or greater than 0.0022 anywhere in the temperature range $1{,}217 < T < 12{,}924$ K were chosen to be species in the extended 'Blake' library.

2. Thermodynamic data for the five permanent gases, N_2, CO, CO_2, H_2, and H_2O were taken from McBride's tables.

3. Thermodynamic data for all of the other species were obtained by expansion of the coefficients in the extended library that McBride had earlier supplied to the ARL.

4. The fitting of these data to the form used by 'Blake' was accomplished using variants of W. H. Zwisler's program, STARFIT, to which various measures of the goodness of fit had been added.

5. The thermodynamic data required for the fittings are the heat capacity as a function of temperature over the desired range, and the enthalpy of formation and the entropy at some reference temperature.

a. In theory the "desired temperature range" could be chosen to extend from 300 K to 10,000 K, but this choice would not be suitable for 'Blake' in general because the available thermodynamic data are limited to compounds of C, H, O, and N. It was deemed more useful to retain the original (old) 'Blake' library for almost all calculations, and to obtain an extended (new) library only for use with ETC formulations (which usually do not contain inorganic additives).

b. In the initial attempts at fitting, 298.15 K was "hard wired" into the program as the reference temperature; the starting temperature was varied from 300 K to 5,000 K. Some fittings were made with a higher reference temperature. They showed that the RMS error of the fit decreased as the reference temperature increased, so the fitting programs were modified to make both the reference temperature and the starting temperature inputs to the program. Survey runs showed that the RMS error was least when these two temperatures were the same.

c. The first of these modified programs, TIGFIT5, which is listed in Appendix K, was used to fit the thermodynamic data for the five permanent gases. The second program, TIGFIT5X, listed in Appendix L, was used for fitting all of the other species. Two programs were used to accommodate the different input formats. It would not have been difficult to adapt one of the programs to accept different input formats, but it was simpler and faster to use different programs.

6. Certain adjustments had to be made in the input files in order to make the comparisons meaningful. Even when limited to C-H-N-O species, there is not a one-to-one correspondence between the two libraries. All in all, there are 17 species that appear only in one or the other of the libraries but not in both. REJect instructions for these 17 species were inserted into all runs in order to ensure that the same species appeared regardless of which library was used.

7. Seven compositions were selected for the comparison:

1) Pseudo M30*
2) JA-2
3) Pseudo M5
4) Pseudo M9
5) M1
6) Decalin + WFNA
7) Decalin + 70% H_2O_2

* *Pseudo* here and elsewhere means that all inorganic additives were omitted from the formulation.

8. The next matter to be settled was the starting temperature (the final temperature would always be 10,000 K).

a. The standard (old) 'Blake' fits cover the range 500 K–5,000 K, and are probably valid somewhat beyond that range, say to 5,500 K. Thus it would be possible to have the extended (new) library start at 5,000 K. Nevertheless it seemed preferable to have it start at a lower temperature.

b. A further requirement was established, that there be little or no difference in results obtained with either library in their overlapping temperature regions. The computed quantities concerned were adiabatic flame temperature, impetus, and ballergy, which is the ratio Impetus/(gamma - 1). Ideally it would have been desirable to make such comparisons for extended libraries with starting temperatures from 2,000 K to 5,000 K, but this was not feasible. Two starting temperatures were selected, 3,000 and 4,000 K. The corresponding libraries were named 30BLKLYB.LIB and 40BLKLYB.LIB, which were used to form the binary libraries 30BLKLYB.DAT and 40BLKLYB.DAT

9. The comparisons were made by plotting the percent differences in the three quantities against the temperature computed by the extended (new) library. The resulting plots for the two libraries were then compared by eye. These plots are shown in Fig-1-A, Fig-1-B, . . . , Fig-1-G. It is readily seen that the better match is found between the standard (old) library and the extended library that starts at 3,000 K. This library was therefore chosen as the final outcome of the present task. The names of the chosen alphanumeric and binary libraries were changed to XBLKLYB.LIB and XBYNLYB.DAT, respectively.

10. As a matter of interest the effect of the REJect instructions was examined by comparing the results with and without them. The resulting plots are shown in Fig-2-A, Fig-2-B, . . . , Fig-2-G. A noticeable difference is found only in the last case. It is caused by the appearance of solid carbon when it is permitted.

V. NBLAKE

A. Although it was not required in the Statement of Work for this task, it seemed appropriate to make some changes and improvements in 'Blake', but the "look and feel" of the program have not been changed.

B. A detailed description of the changes is given in the documentation for the revised program. The principal changes concern the library; the net result is that the new library is incompatible with all previous versions of the program, and previous versions of the program are incompatible with the new library. This change was made deliberately in order to improve the paper trail leading from output back to the library on which it was based.

INTENTIONALLY LEFT BLANK.

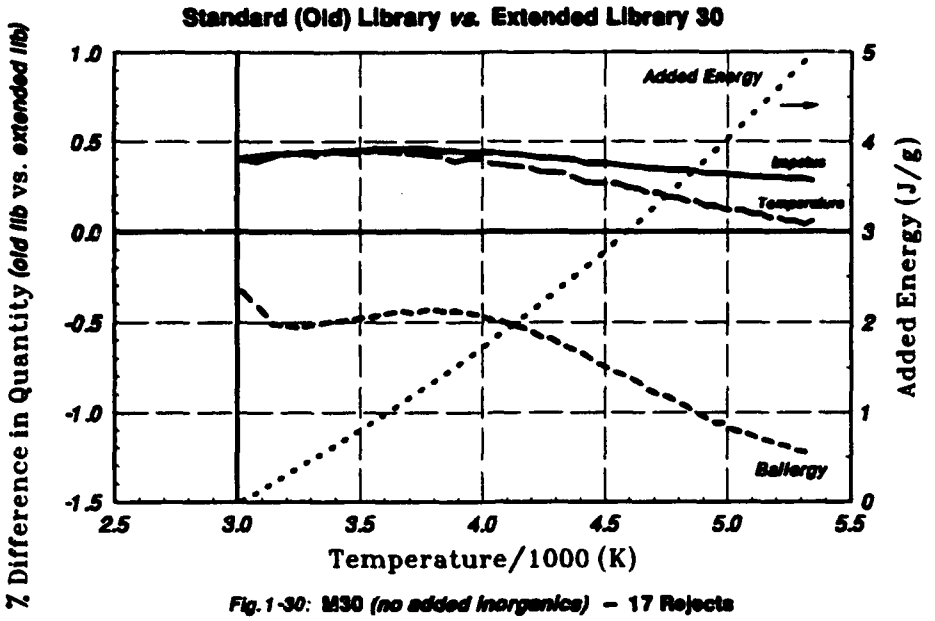

Fig. 1-30: M30 *(no added inorganics)* – 17 Rejects

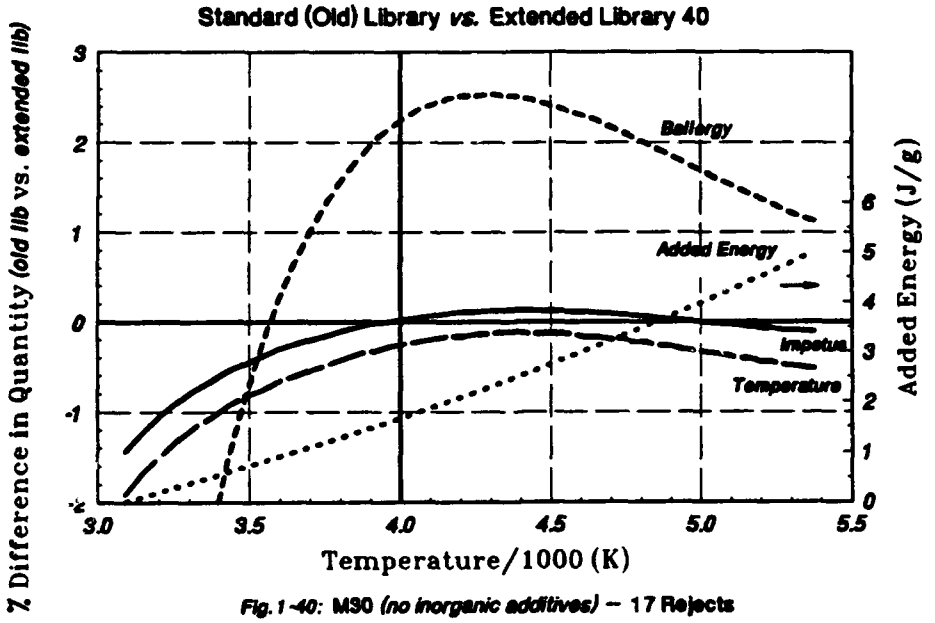

Fig. 1-40: M30 *(no inorganic additives)* – 17 Rejects

Figure 1-A: **M30** ***(no inorganic additives)*** **-- 17 Rejects**

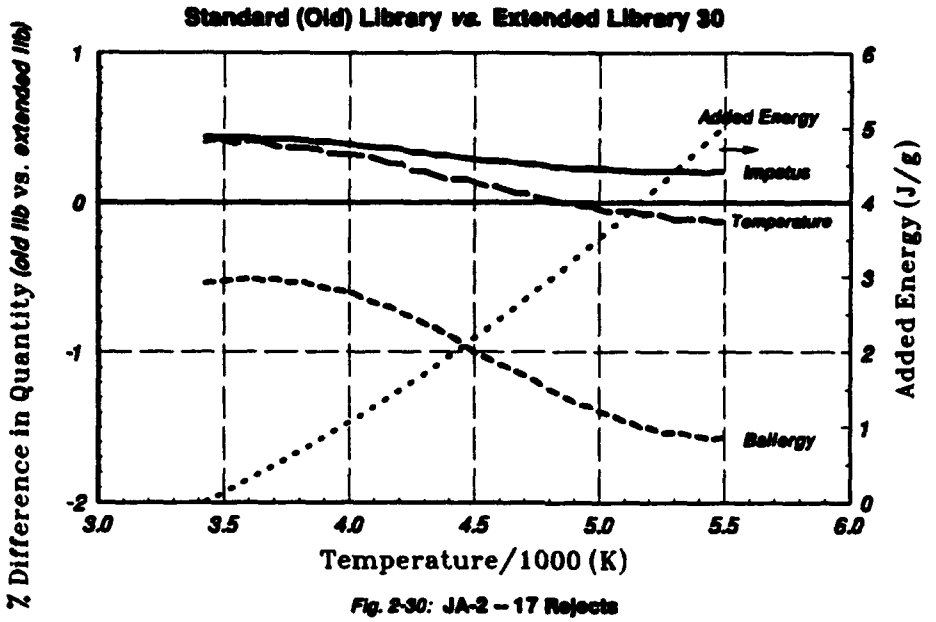

Fig. 2-30: JA-2 – 17 Rejects

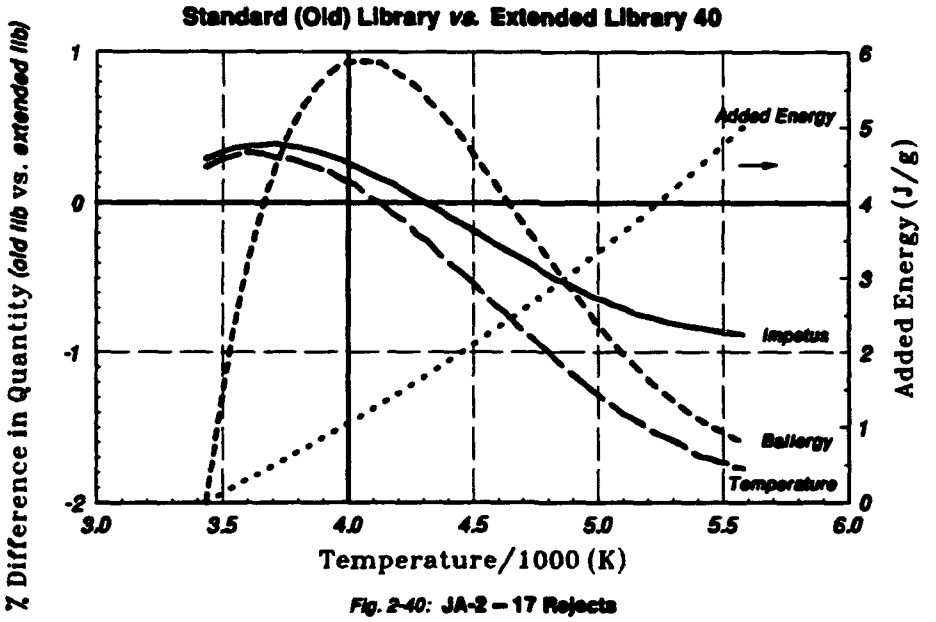

Fig. 2-40: JA-2 – 17 Rejects

Figure 1-B: JA-2 -- 17 Rejects

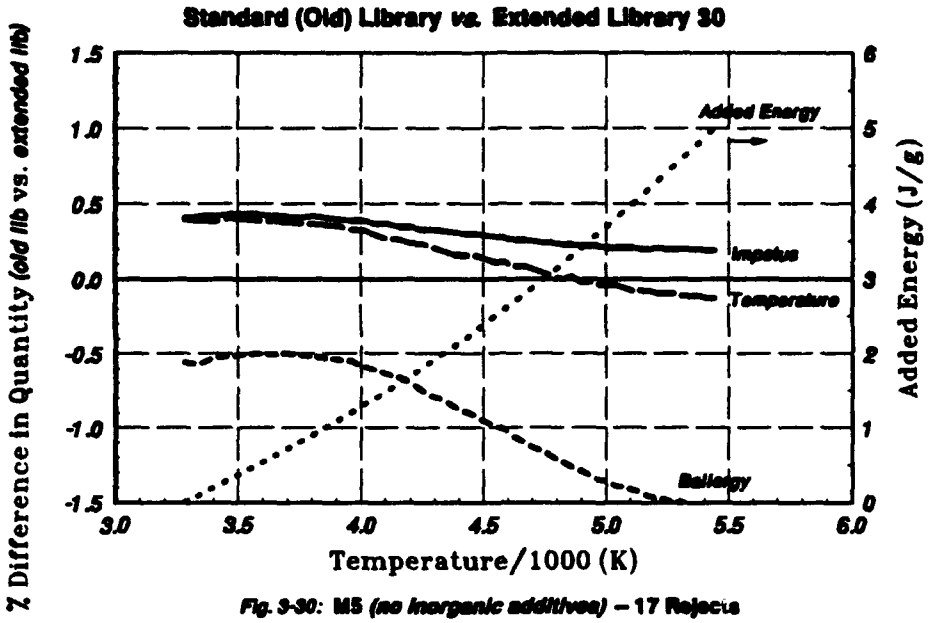

Fig. 3-30: M5 *(no inorganic additives)* – 17 Rejects

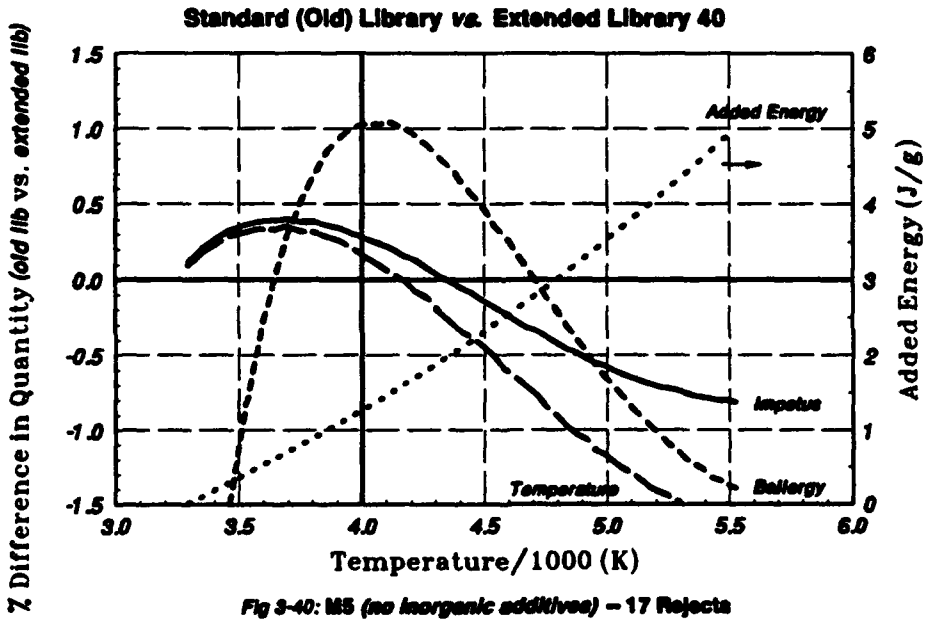

Fig 3-40: M5 *(no inorganic additives)* – 17 Rejects

Figure 1-C: M5 *(no inorganic additives)* -- 17 Rejects

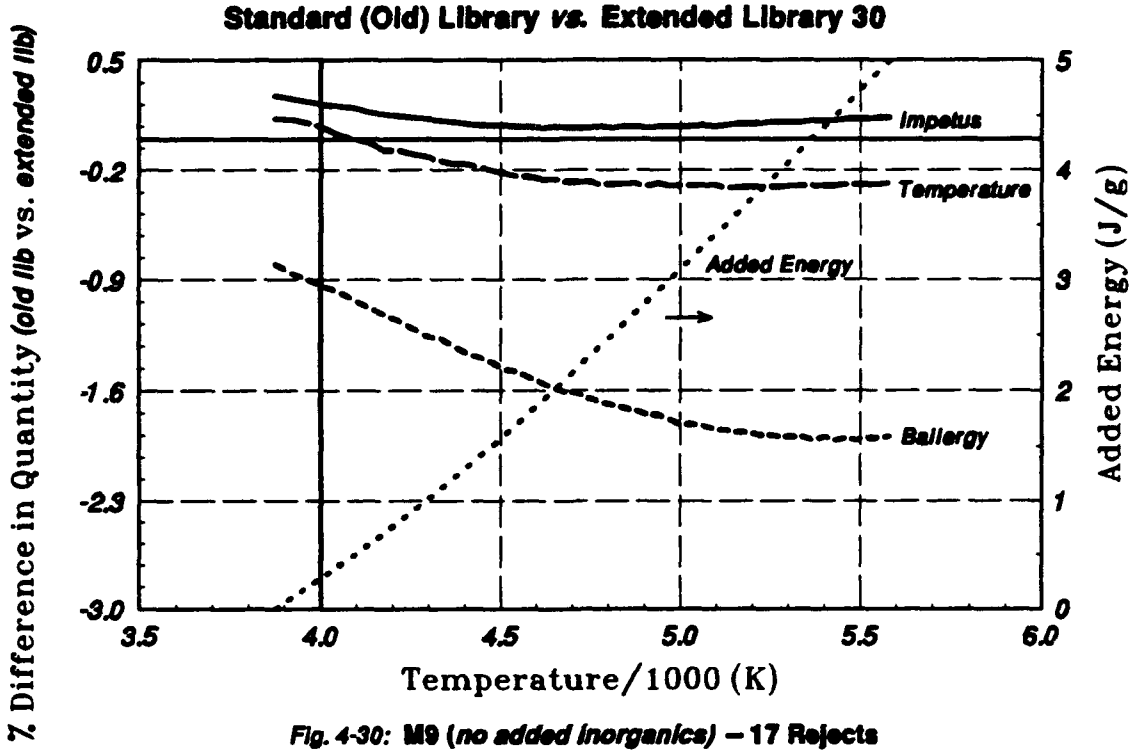

Fig. 4-30: **M9 (*no added inorganics*) – 17 Rejects**

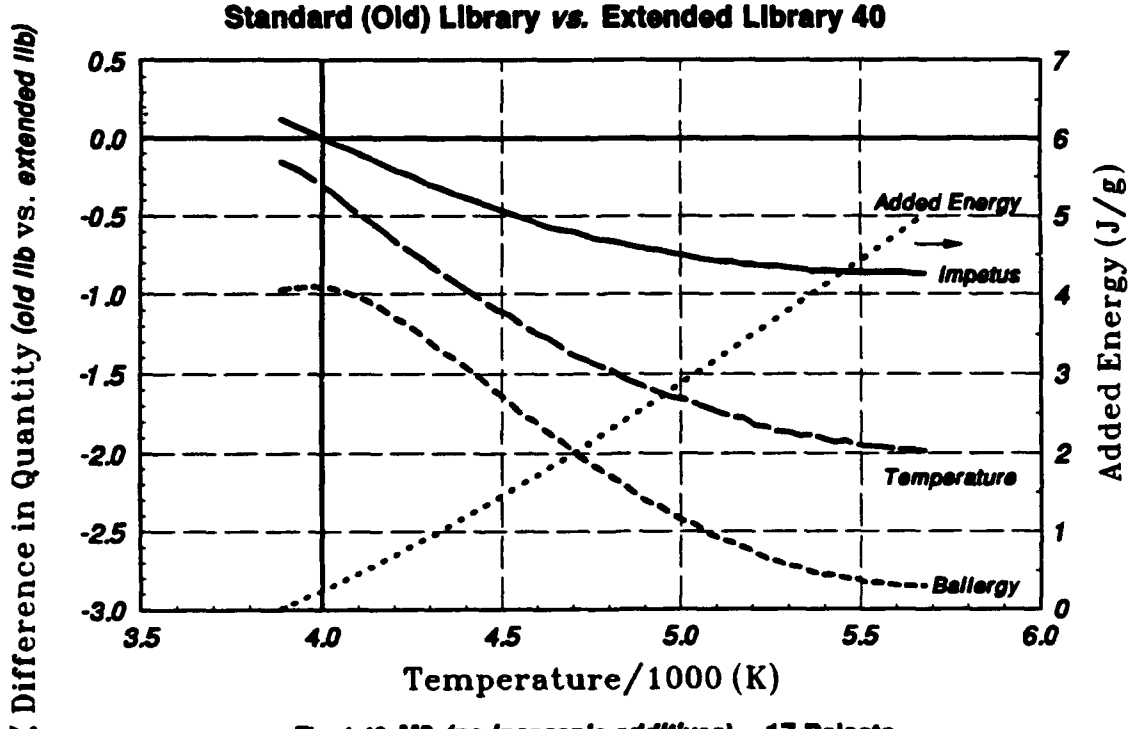

Fig. 4-40: **M9 (*no inorganic additives*) – 17 Rejects**

Figure 1-D: **M9 *(no inorganic additives)* -- 17 Rejects**

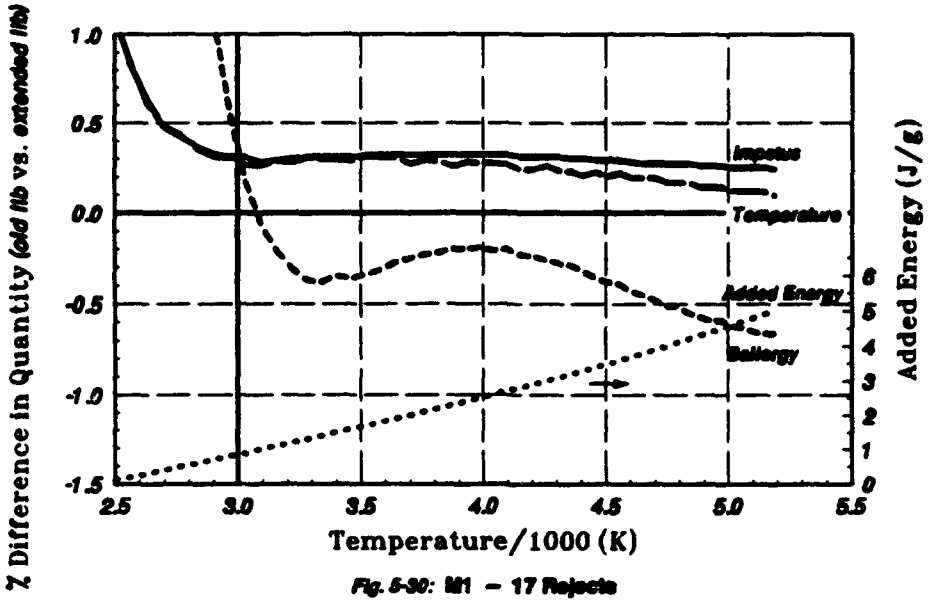

Fig. 5-30: M1 – 17 Rejects

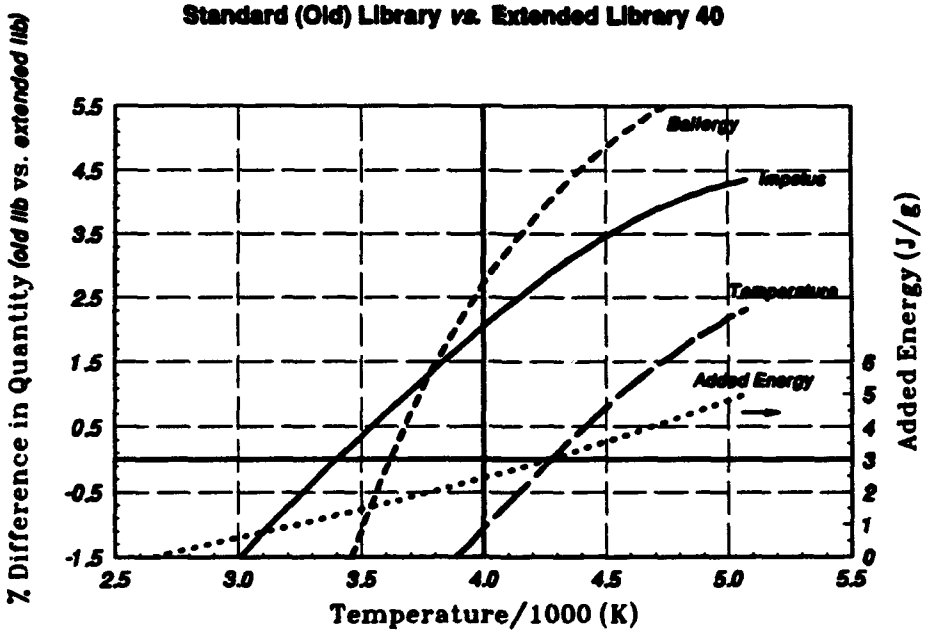

Fig. 5-40: M1 – 17 Rejects

Figure 1-E: **M1 -- 17 Rejects**

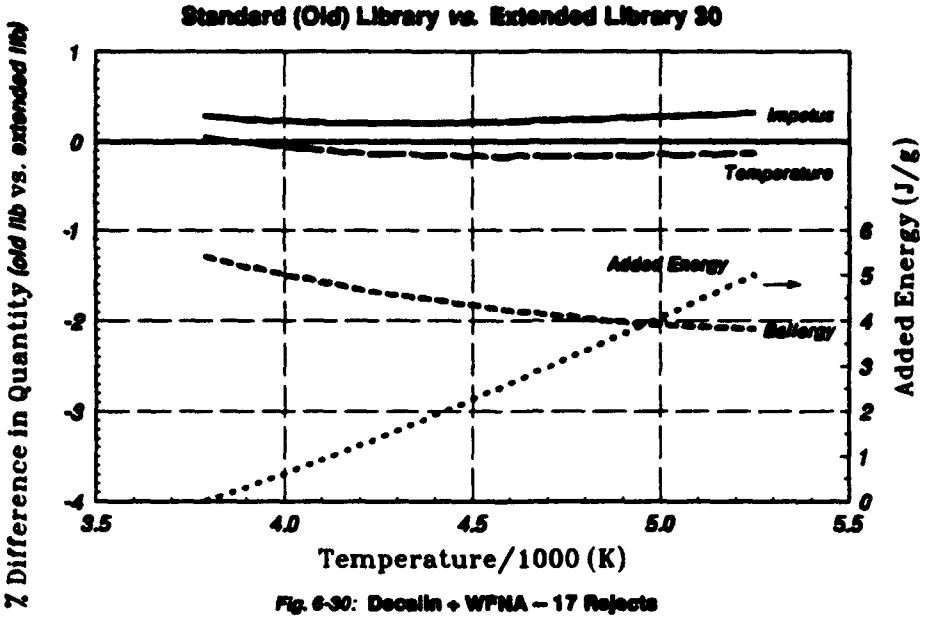

Fig. 6-30: Decalin + WFNA – 17 Rejects

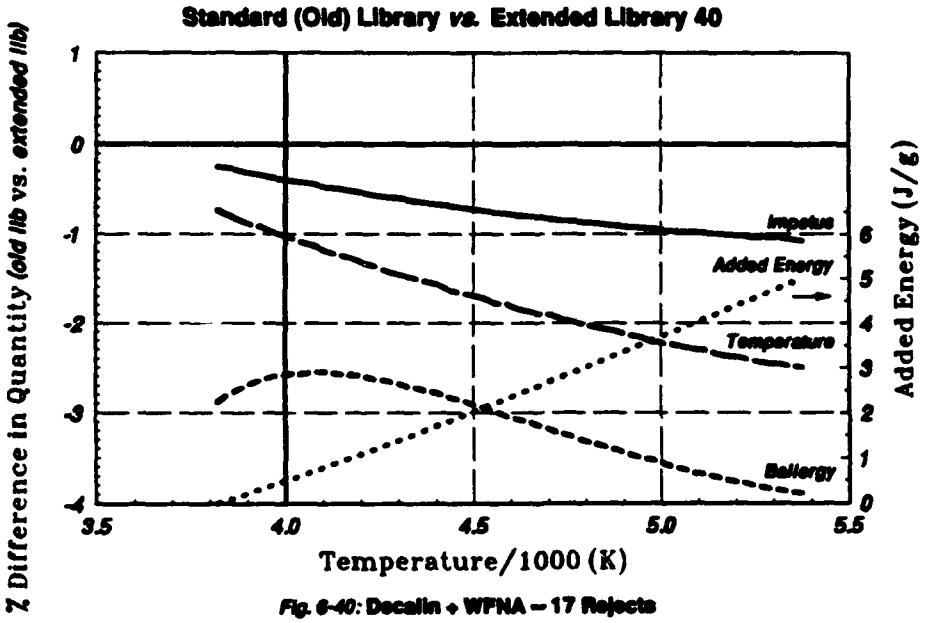

Fig. 6-40: Decalin + WFNA – 17 Rejects

Figure 1-F: **Decalin + WFNA -- 17 Rejects**

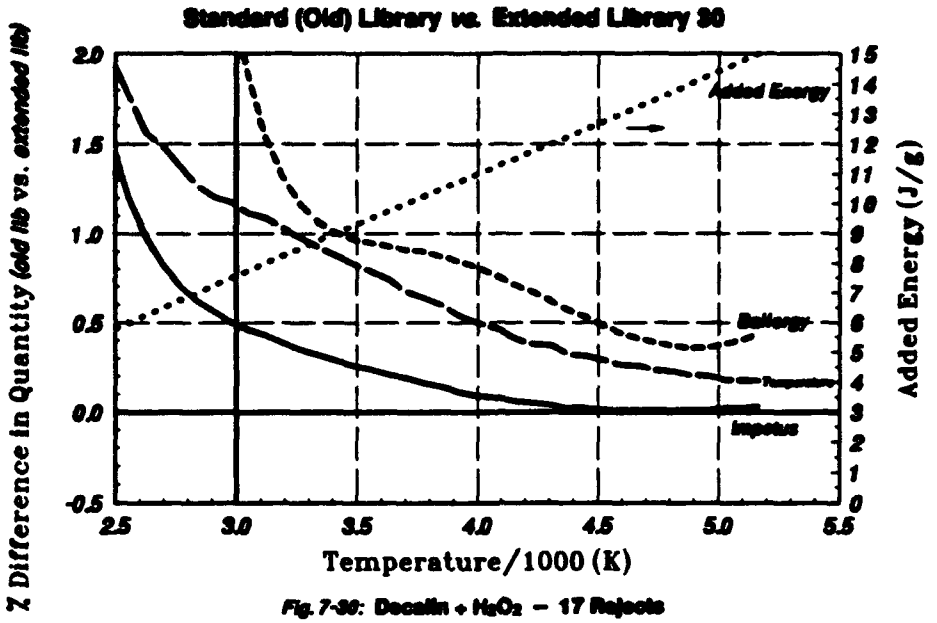

Fig. 7-30: Decalin + H_2O_2 – 17 Rejects

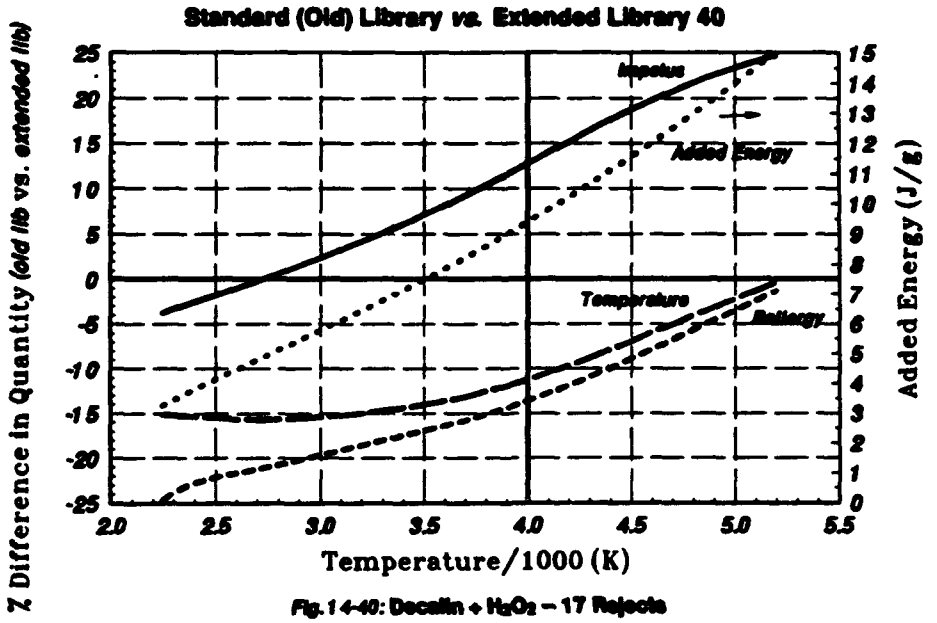

Fig. 14-40: Decalin + H_2O_2 – 17 Rejects

Figure 1-G: Decalin + H_2O_2 -- 17 Rejects

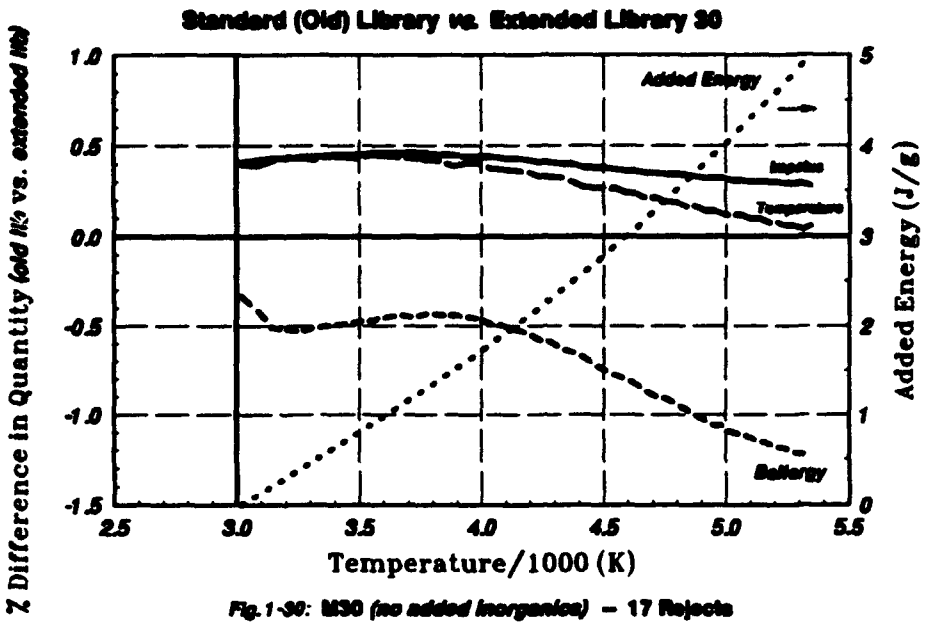

Fig. 1-30: M30 (no added inorganics) – 17 Rejects

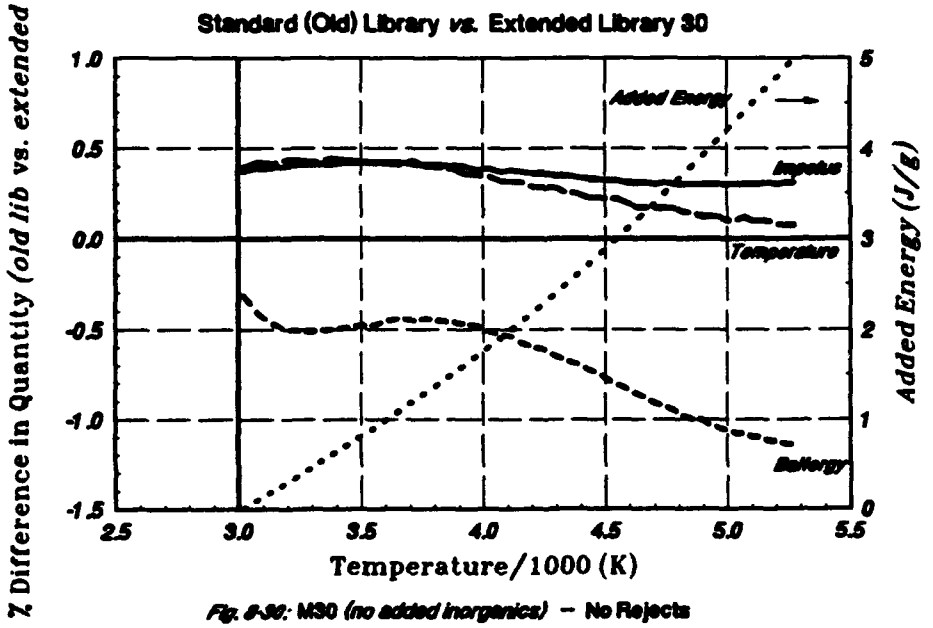

Fig. 2-30: M30 (no added inorganics) – No Rejects

Figure 2-A: M30 *(no inorg additives)* -- Rejects *vs.* No Rejects

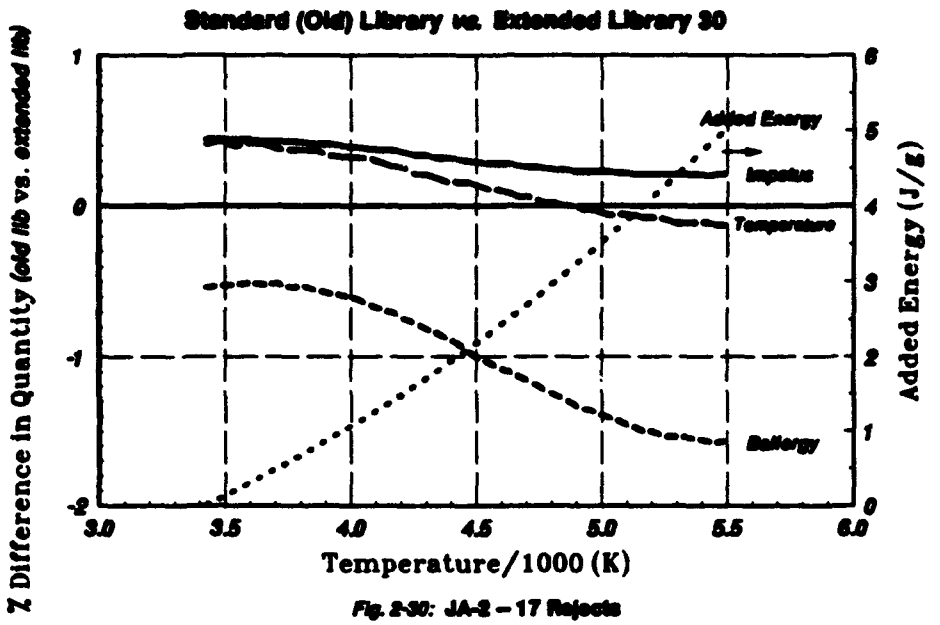

Fig. 2-30: JA-2 – 17 Rejects

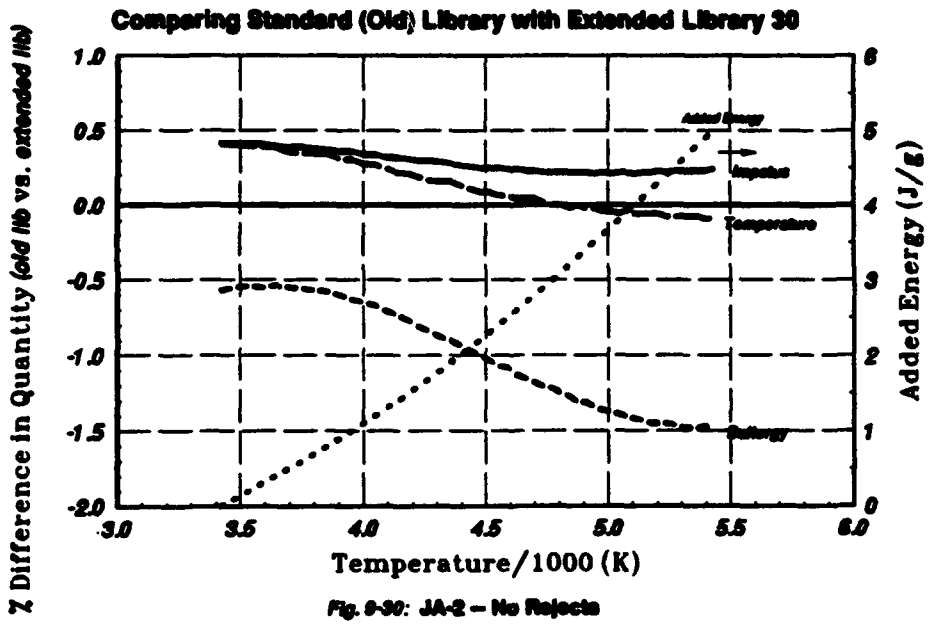

Fig. 2-30: JA-2 – No Rejects

Figure 2-B: JA-2 -- 17 Rejects *vs*. No Rejects

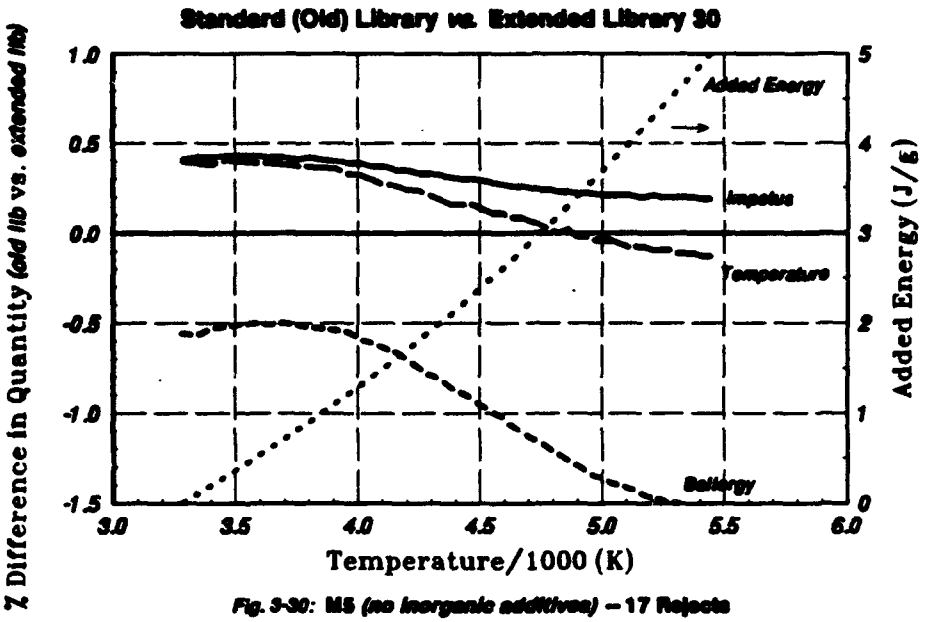

Fig. 3-30: M5 (no inorganic additives) -- 17 Rejects

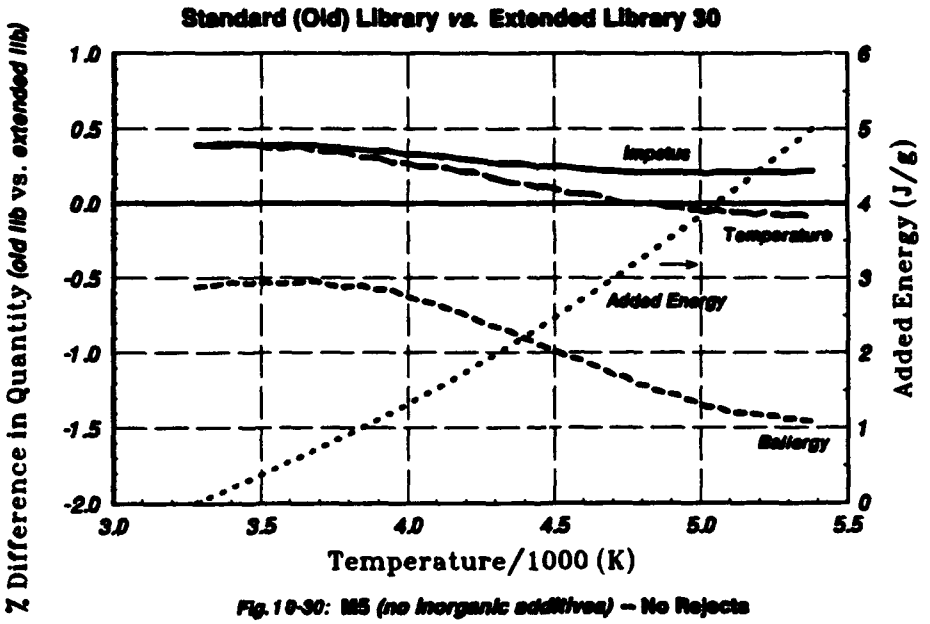

Fig. 19-30: M5 (no inorganic additives) -- No Rejects

Figure 2-C: M5 *(no inorg additives)* -- 17 Rejects *vs* No Rejects

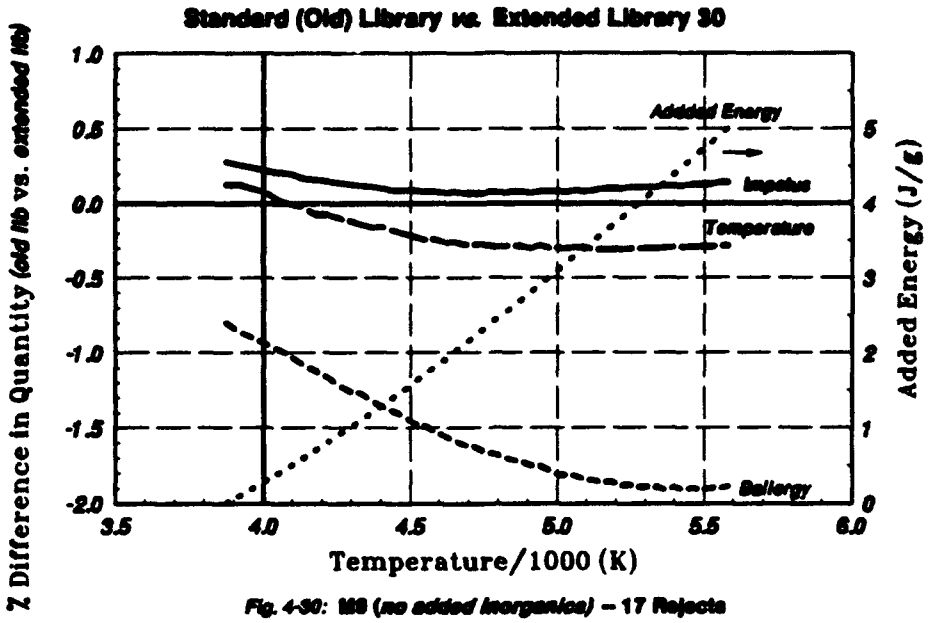

Fig. 4-30: M9 (no added inorganics) – 17 Rejects

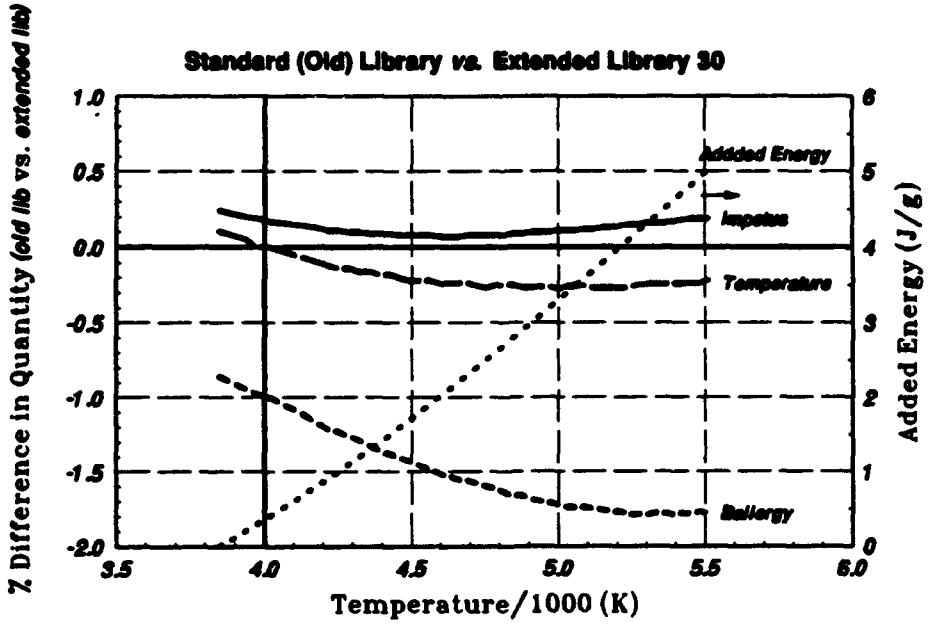

Fig. 11-30: M9 (no inorganic additives) – No Rejects

Figure 2-D: M9 *(no inorg additives)* -- 17 Rejects *vs* No Rejects

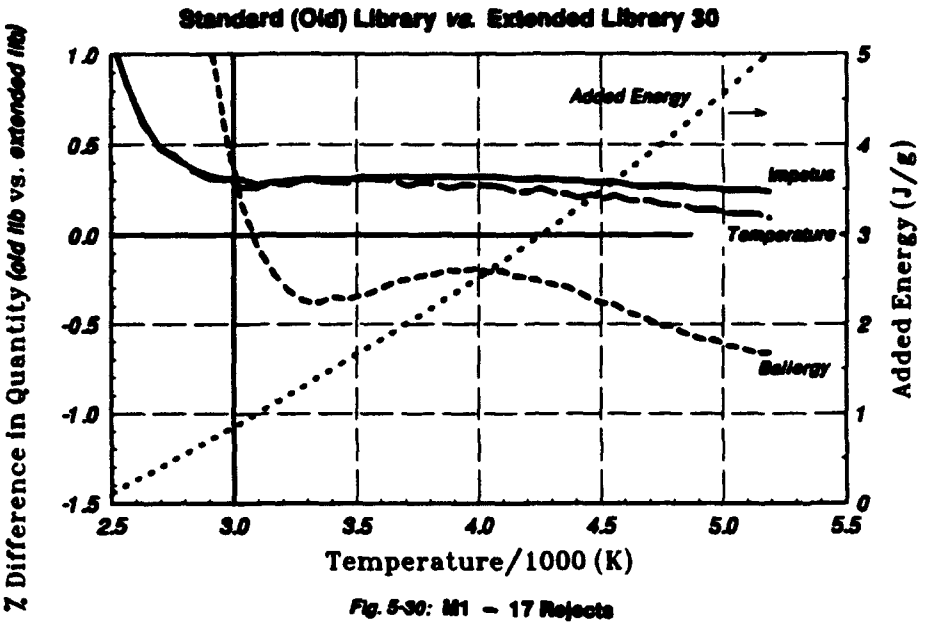

Fig. 5-30: M1 – 17 Rejects

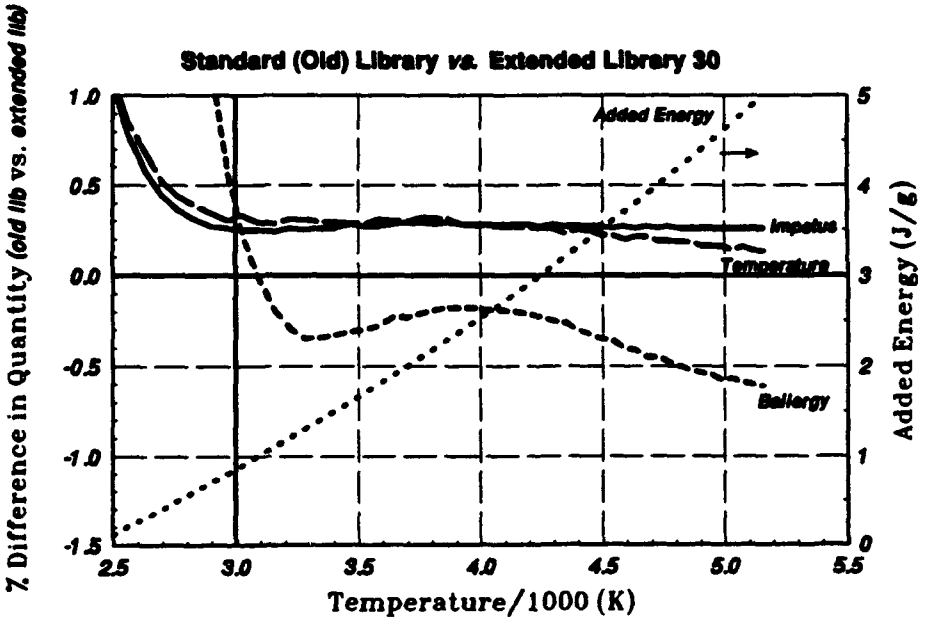

Fig. 12-30: M1 – No Rejects

Figure 2-E: **M1 -- 17 Rejects *vs* No Rejects**

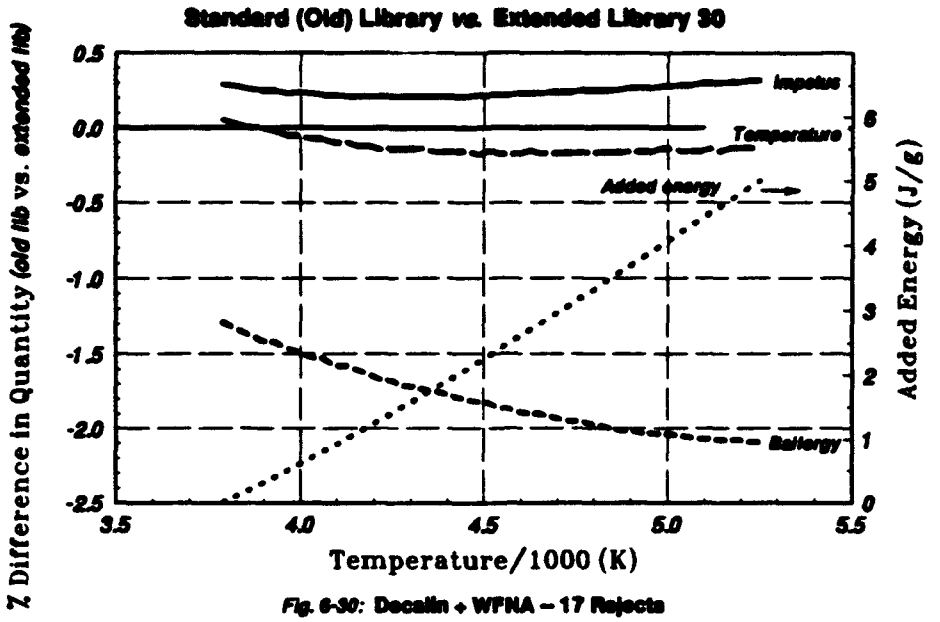

Fig. 6-30: **Decalin + WFNA – 17 Rejects**

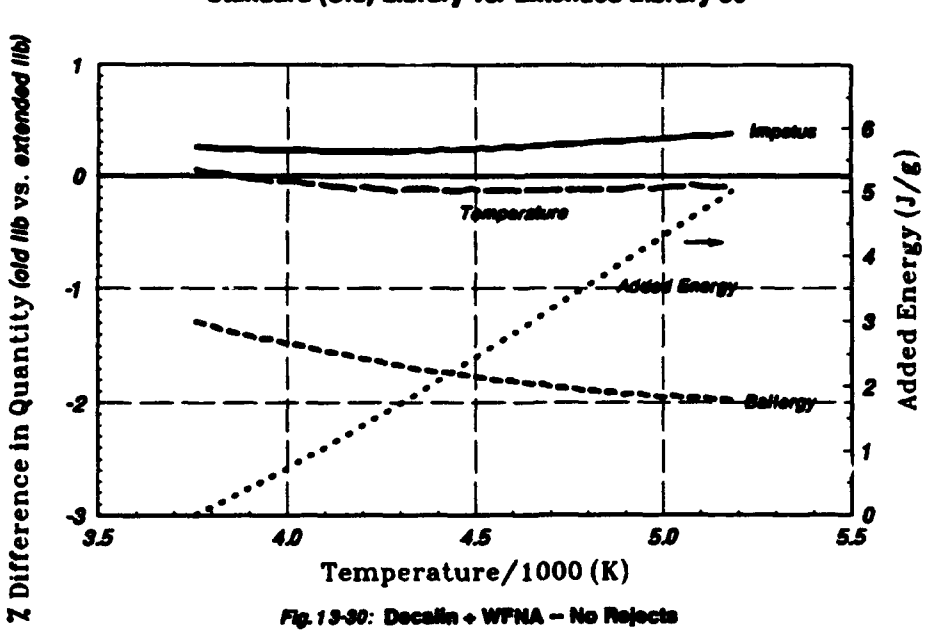

Fig. 13-30: **Decalin + WFNA – No Rejects**

Figure 2-F: **Decalin + WFNA -- 17 Rejects *vs* No Rejects**

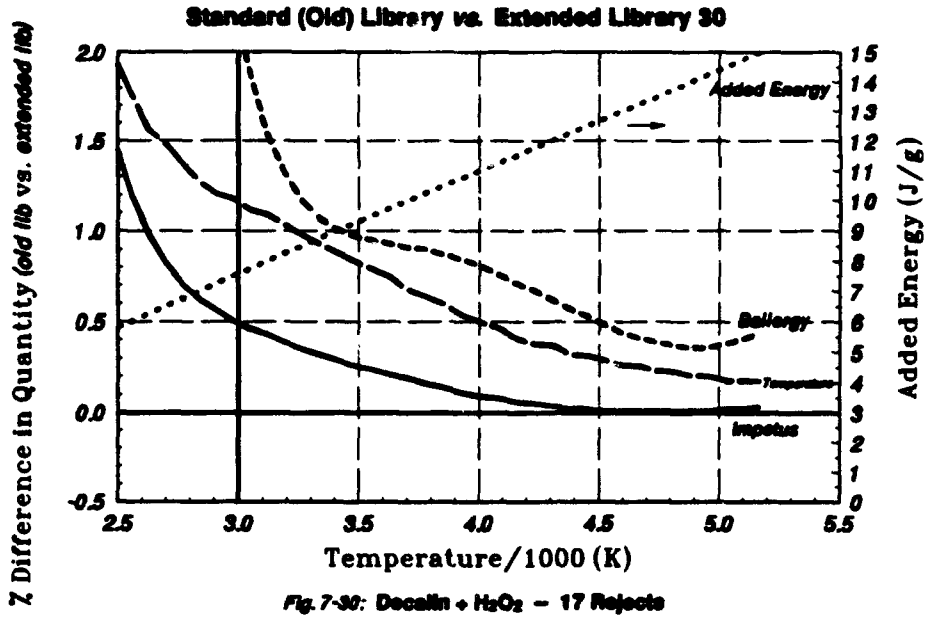

Fig. 7-30: Decalin + H_2O_2 – 17 Rejects

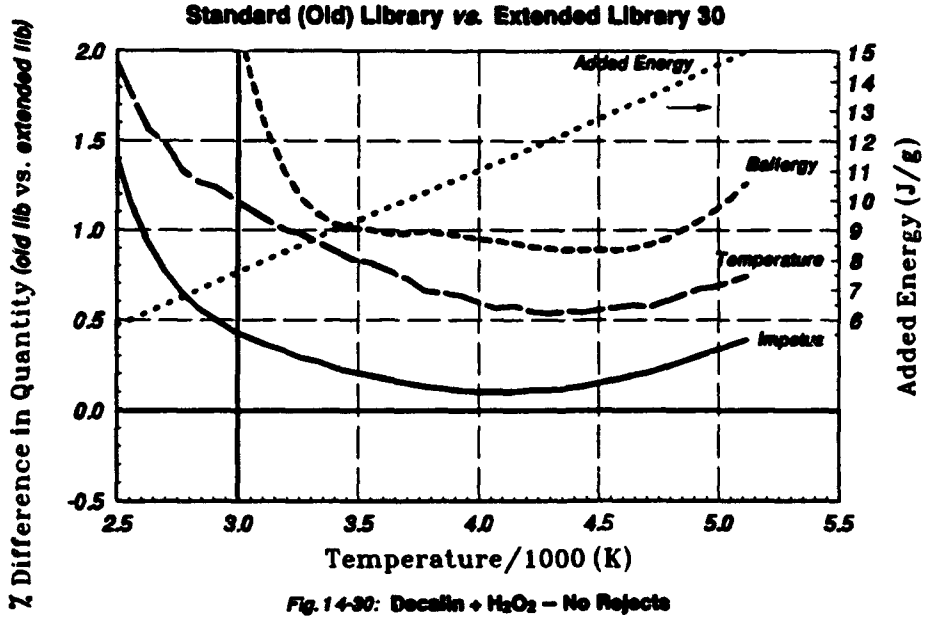

Fig. 14-30: Decalin + H_2O_2 – No Rejects

Figure 2-G: Decalin + H_2O_2 -- 17 Rejects *vs* No Rejects

Appendix A.

Listing of TESTLIBS.BAT

```
REM A batch file to compare old & new McBride libraries up to 6,000 K
@ECHO Off

rem 11 September 1992

rem  This batch file runs EXMUCET for 4 cases:
rem      o  without or with ions permitted, and
rem      o  using old (standard) and new (extended) thermo libraries.
rem  The following 8 files are produced:
rem      o  tstlbsno.old and tstlbsio.old  (summary w/ old lib )
rem                ^no ions          ^ions
rem      o  tstlbono.old and tstlboio.old  (output  "  "   "  )
rem      o  tstlbsno.new and tstlbsio.new  (summary w/ new lib )
rem      o  tstlbono.new and tstlboio.new  (output  "  "   " )
rem  Then the summary files are operated on by COMPARE2.BAS, producing:
rem      o  summary1.tab: compares no ions/ions & old library;
rem      o  summary2.tab: compares no ions/ions & new library;
rem      o  summary3.tab: compares old & new libraries, no ions;
rem      o  summary4.tab: compares old & new libraries, with ions;

rem Start timer
c:\norton\tm start start /log /l
echo.
rem Is only a comparison wanted?
if "%1" == "Q" goto quikk
rem Verify whether new binary libraries are to be created
if "%1" == "" goto RUN1
if "%1" == "C" goto makelib
if not "%1" == "c" goto RUN1
:MAKELIB
cls
echo.
echo.
echo      Confirm that you want a CREATION run, or press ^C to abort:
echo.
pause
rem    Start with standard FILE4.DAT; convert it to new format
echo.
echo              Copying standard FILE4.DAT to EXFILE4.DAT
copy d:\cet\source\library\file4.dat file4.dat > nul:
echo.
echo                    Converting FILE4.DAT to INTFILE.DAT
@echo on
oldint file4.dat
@echo off
```

```
echo.
echo                    Converting INITFILE.DAT to NEWFILE.DAT
@echo on
intnew
@echo off
echo.
echo    Add identifying header to NEWFILE.DAT
copy old_lib.hed + newfile.dat tempo > nul:
del newfile.dat
ren tempo newfile.dat
echo.
echo                    Now form binary library
copy lib_run.in input > nul:
@echo on
exmucet newfile.dat
del newfile.dat
del intfile.dat
del file4.dat
@echo off
echo.
echo              Save binary library for future use.
copy exthrmlb.dat newstd.lib > nul:

rem    Now repeat with McBride's extended library
echo.
echo           Copying McBride's extended FILE4.DAT to EXFILE4.DAT

copy d:\cet\source\library\exfile4.dat exfile4.dat > nul:
echo.
echo                    Now form binary library

copy lib_run.in input > nul:
@echo on
exmucet exfile4.dat
@echo off
echo.
echo              Save binary library for future use.

copy exthrmlb.dat exfile4.lib > nul:
goto run2

:RUN1
cls
echo.
REM  echo   Confirm NO need to (re)create libraries, or press ^C to abort
echo.
REM   pause
rem      Start here if libraries have previously been formed
:RUN2
```

```
echo              Copy standard binary libary to EXTHRMLB.DAT
copy newstd.lib exthrmlb.dat > nul:
echo Copy first set of test cases to INPUT
copy \cet\exform\no_ions.in input > nul:
echo.
echo                    ...and now run EXMUCET using OLD library
echo.
@echo on
exmucet
@echo off
echo.
echo                    Save output

copy summary tstlbsno.old > nul:
copy output  tstlbono.old > nul:

echo.
echo  Now copy new set of test cases (thermo library unchanged)
echo.
echo.    Copying ions.in to input
copy ions.in input > nul:
echo.
echo Now re-run EXMUCET
@echo on
exmucet
@echo off
echo.
echo                    Save output

copy summary tstlbsio.old > nul:
copy output  tstlboio.old > nul:
rem    Now repeat these calculations using McBride's extended library
echo.
echo                Copy previously-formed new binary library
copy exfile4.lib exthrmlb.dat > nul:
echo.
echo  Run the same test file again
echo.
exmucet
@echo off
echo.
echo              Save output for comparison

copy  output tstlboio.new > nul:
copy summary tstlbsio.new > nul:

echo.
echo     Copy FIRST test of test cases...
echo.
```

```
copy no_jons.in input > nul:
echo.
echo          ... and run EXMUCET
exmucet
@echo off
echo.
echo             Save output for comparison

copy output  tstlbono.new > nul:
copy summary tstlbsno.new > nul:
rem   Stop timer
c:\norton\tm stop done /l > dummy
c:\norton\tm stop done /l
copy dummy d:\cet\exform\time_run > nul:
del dummy
echo.
echo  Delete scratch files (if any)
del zz*.*
:quikk
echo.
echo. Run COMPARE.BAS 4 times
echo.
copy testlib1.in test_opt > nul:
qb/run \cet\exform\source\compare
copy summary.tab summary1.tab > nul:
copy testlib2.in test_opt > nul:
qb/run \cet\exform\source\compare
copy summary.tab summary2.tab > nul:
copy testlib3.in test_opt > nul:
qb/run \cet\exform\source\compare
copy summary.tab summary3.tab > nul:
copy testlib4.in  test_opt > nul:
qb/run \cet\exform\source\compare
copy summary.tab summary4.tab > nul:

if "%1" == "Q" goto qq
echo.
echo  For safety's sake, ensure that EXTHRMLB.DAT is (new) extended library
copy exfile4.lib exthrmlb.dat > nul:
echo.

:qq
if "%1" == "Q" call wdstar d:\cet\exform\summary3.tab
if "%1" == "Q" goto endd

call wdstar d:\cet\exform\time_run
:endd
d:
cd\cet\exform
```

Appendix B.

Listing of PROGRAM MAKE_INP.BAS

NOTE: In order to improve the legibility of the listings of the QUICK BASIC programs given in this report, the underscore, '_', has been used as a continuation symbol in some lines that would otherwise be too long.

EXAMPLE: A line such as

```
PRINT #2, num.kase2(kase); ","; temp2(kase); ","; gmptus2(kase); ","
```

will be printed here as

```
PRINT #2, num.kase2(kase); ","; temp2(kase); ","; _
                gmptus2(kase); ","
```

```
' A program to make huge run streams for checking EXMUCET
' Written by EF&A in Aug/92
' Saved as MAKE_INP.BAS [5 September 1992]

DIM e.zero(15)
DEFINT I-N: DEFSNG A-H, O-Z

DATA -1538.79 , -1587.72 , -2488.30 , -2302.44, -2103.22
DATA -2316.85 , -2625.75 , -5145.85 , -1573.22
DATA -99999., 0, 0, 0, 0 , 0

FOR i = 1 TO 15: READ e.zero(i): IF (e.zero(i) = -99999!) THEN num.e = i - 1
NEXT

CLS : FOR i = 1 TO 7: PRINT : NEXT
INPUT "Enter in order: E start, Delta E, and E final: ", _
                        energyz, delta.e, e.final

FOR k.inp = 1 TO 2
   CLOSE #1: CLOSE #2
   IF (k.inp = 1) THEN
        file.inputt$ = "d:\cet\exform\template.1"
        file.output$ = "d:\cet\exform\no_ions.in"
   ELSE
        file.inputt$ = "d:\cet\exform\template.2"
        file.output$ = "d:\cet\exform\ions.in"
   END IF
OPEN file.output$ FOR OUTPUT AS #2:

energy = 0!
```

```
recycle: OPEN file.input$ FOR INPUT AS #1
IF (energy <> 0!) THEN GOTO start
PRINT "              ";
FOR i = 1 TO INT(1.05 * e.final / delta.e + 1): _
                    PRINT enerzy + delta.e * (i - 1); ","; : NEXT:
PRINT
PRINT #2, "              ";
FOR i = 1 TO INT(1.05 * (e.final / delta.e) + 1): _
                PRINT #2, enerzy + delta.e * (i - 1); ",";
                                NEXT: PRINT #2, " "
PRINT #2, "              -9999."
energy = enerzy
start:  kk = 0
read1: LINE INPUT #1, lyne$: IF (EOF(1)) THEN GOTO new.energy
     FOR i = 1 TO LEN(lyne$)
       IF (MID$(lyne$, i, 1) = "#") THEN
         num = i - 1: GOSUB makeline1: GOTO read2
       END IF
     NEXT
'       print lyne$
      PRINT #2, lyne$: GOTO read1
read2: LINE INPUT #1, lyne$
     FOR i = 1 TO LEN(lyne$)
       IF (MID$(lyne$, i, 2) = "U=" AND MID$(lyne$, i + 2, 1) = "#") THEN
         num = i - 1: GOSUB makeline2: GOTO read1
       END IF
     NEXT
'          print lyne$
          PRINT #2, lyne$: GOTO read2

new.energy: energy = energy + delta.e: PRINT "Energy = "; energy
   IF (energy > e.final) THEN
        GOTO nexxt2
   ELSE
        CLOSE #1: GOTO recycle
   END IF
nexxt2: NEXT
SYSTEM

makeline1:
' a subroutine to insert the added energy into the title line
     dum$ = LEFT$(lyne$, num)
     dum$ = dum$ + STR$(energy) + " J/g Elec": PRINT #2, dum$:
                              PRINT dum$: RETURN
makeline2:
' a subroutine to insert the revised energy into the namelist line
     kk = kk + 1
     dum$ = LEFT$(lyne$, num)
     dum$ = dum$ + "U=" + STR$(energy + e.zero(kk)) + "/"
```

```
PRINT #2, dum$:
PRINT dum$
RETURN
```

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Appendix C.

Template of the Test Cases for Comparing

Different Thermodynamics Libraries

```
TITLE
1. Pseudo M30 -- NO IONS ALLOWED + # J/g Added

REACTANTS
C 6.      H 7.549    O 9.901    N 2.451          27.90    -169.16E3S298.15    F
C 3.      H 5.       O 9.       N 3.             22.42    -8.86E4  S298.15    F
C 1.      H 4.       N 4.       O 2.             47.54    -2.21E4  S298.15    F
C 17.     H 20.      N 2.       O 1.              1.49    -2.51E4  S298.15    F
C 1.                                              .10     0.0      S298.15    F
C 2.      H 6.       O 1.                         .25     -66.42E3L298.15     F

NAMELISTS
 &INPT2  UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/

TITLE
2. M30A1 -- NO IONS ALLOWED + # J/g Added

REACTANTS
C 6.      H 7.739    O 9.521    N 2.261          27.9     -173.77E3S298.15    F
C 3.      H 5.       O 9.       N 3.             22.42    -88.6E3  L298.15    F
C 1.      H 4.       O 2.       N 4.             46.84    -22.1E3  S298.15    F
C 17.     H 20.      O 1.       N 2.              1.49    -25.1E3  S298.15    F
C 2.      H 6.       O 1.                         .25     -66.42E3 L298.15    F
C 1.                                              .1      0.       S298.15    F

NAMELISTS
 &INPT2  UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/

TITLE
3. Pseudo WC890 -- NO IONS ALLOWED + # J/g Added

REACTANTS
C 6.      H 7.549    O 9.901    N 2.451          79.98    -169.16E3S298.15    F
C 3.      H 5.       O 9.       N 3.             10.2     -8.86E4  S298.15    F
C 12.     N 1.       H 11.                       1.11     3.107E4  S298.15    F
C 16.     H 22.      O 4.                        7.65     -201.E3  S298.15    F
C 7.      H 6.       O 4.       N 2.              .08     -1.71E4  S298.15    F
C 1.                                              .14     0.0      S298.15    F

NAMELISTS
 &INPT2  UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/
```

TITLE
4. JA-2 (FRG) -- NO IONS ALLOWED + # J/g Added

REACTANTS

C 6.	H 7.395	O 10.209	N 2.605	59.5	-165.41E3S298.15	F
C 3.	H 5.	O 9.	N 3.	14.9	-88.6E3 L298.15	F
C 4.	H 8.	O 7.	N 2.	24.8	-103.56E3S298.15	F
C 2.	H 6.	O 1.		.05	-66.42E3 L298.15	F
C 14.	H 14.	N 2.	O 1.	.7	-255.E3 L298.15	F

NAMELISTS
&INPT2 UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=# /

TITLE
5. M9 -- NO IONS ALLOWED + # J/g Added

REACTANTS

C 6.	H 7.329	O 10.341	N 2.671	57.55	-163.81E3S298.15	F
C 3.	H 5.	O 9.	N 3.	39.86	-88.6E3 L298.15	F
C 17.	H 20.	O 1.	N 2.	.75	-25.1E3 S298.15	F
C 2.	H 6.	O 1.		.35	-66.42E3 L298.15	F

NAMELISTS
&INPT2 UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/

TITLE
6. M1 -- NO IONS ALLOWED + # J/g Added

REACTANTS

C 6.	H 7.364	O 10.271	N 2.636	83.11	-164.65E3S298.15	F
C 7.	H 6.	O 4.	N 2.	9.77	-17.1E3 S298.15	F
C 16.	H 22.	O 4.		4.89	-201.4E3 L298.15	F
C 2.	H 6.	O 1.		.05	-66.42E3 L298.15	F
C 12.	H 11.	N 1.		.98	31.07E3 L298.15	F
H 2.	O 1.			.50	-285831. L298.15	JF

NAMELISTS
&INPT2 UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/

TITLE
7. DECALIN + WFNA -- NO IONS ALLOWED + # J/g Added

REACTANTS

H 1.	N 1.	O 3.	.8088	-41.61E3 L298.15	F
C 10.	H 18.		.178	-55.1E3 L298.15	F
N 1.	O 2.		.02466	31711. G298.15	JF
H 2.	O 1.		.010686	-285831.L298.15	JF

```
NAMELISTS
 &INPT2  UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/

TITLE
8. DECALIN + 70% HYDROGEN PEROXIDE -- NO IONS ALLOWED + # J/g Added

REACTANTS
C 10.    H 18.                                  1.     -55.1E3  L298.15     F
H 2.     O 2.                                   .7     -44.88E3 L298.15     O
H 2.     O 1.                                   .3     -68.315E3L298.15     O

NAMELISTS
 &INPT2  UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/

TITLE
9. RFNA + UDMH -- NO IONS ALLOWED + # J/g Added

REACTANTS
N        1.6294   H 1.5722   O 4.6950           .7     -64860.  L298.15     F
C 2.     H 8.     N 2.                         .3     11.9E3   L298.15     F

NAMELISTS
 &INPT2  UV=T,RHO=0.2, SIUNIT=T,IONS=F,U=#/

STOP
```

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Appendix D.

Listing of Program COMPARE.BAS

```
' A program to compare output files from EXMUCET
' Written by EF&A in Oct/92

' Saved as D:\EXMUCET\COMPARE.BAS
' This version: 01-MAR-1994
'    -- Error in file names in DATA statement corrected
'    -- Changes begun on 13-FEB-94 made internally consistent & completed.
'    -- Some cosmetic changes made.

' 13 February 1994:
' On-screen directions added.
' Use of external file for options discarded.
' File names changed.

' 9 February 1994:
' File names changed

' Modified [27-OCT-93] to remove bugs and to simplify the programming;
' The output was improved.

' Modified [11-SEP-92] to include identification of the thermo
'  libraries used to generate the outputs being compared.

CLS : DEFINT I-N: DEFSNG A-H, O-Z
DIM temp1(999), gmptus1(999), ballergy1(999)
DIM num.kase1(999), num.kase2(999), e.zero(99)
DIM temp2(999), gmptus2(999), ballergy2(999)
DIM Delta.g(999), Delta.pct.t(999), Delta.pct.b(999)
DIM Delta.t(999), Delta.b(999)
energy.save = -1!: no.ener = 0: no.cmpsns = 8

' Determine type of run.  There are 3 types: Compare results from
' McBride's standard library without ions or with ions permitted, and
' compare the standard library with the extended one without or with
' ions permitted.

get.option:
COLOR 1, 11: CLS : LOCATE 3, 7
PRINT " "; : COLOR 1, 7: PRINT "TYPE 1"; : COLOR 1, 11
PRINT "  Compare results from the standard library with        "
PRINT SPACE$(17); "results from the extended library, no ions permitted."
```

```
LOCATE 6, 7
PRINT " "; : COLOR 1, 7: PRINT "TYPE 2"; : COLOR 1, 11
PRINT "  Compare results from the standard library with        "
PRINT SPACE$(17); "results from the extended library, ions permitted."

LOCATE 9, 7
PRINT " "; : COLOR 1, 7: PRINT "TYPE 3"; : COLOR 1, 11
PRINT "  Compare results from the extended library             "
PRINT SPACE$(17); "without or with ions permitted."

LOCATE 14, 17: COLOR 15, 9: PRINT "Enter your option 1, 2, or 3: "
waitt:
a$ = INKEY$: IF (LEN(a$) = 0) THEN GOTO waitt
CLS : opt = VAL(a$)
IF (opt < 1 OR opt > 3) THEN CLS : PRINT CHR$(7): GOTO get.option

COLOR 15, 5: LOCATE 9, 25: PRINT " Option chosen ="; opt
LOCATE 11, 19:                PRINT " WAIT.  Data are being processed. "
COLOR 15, 9
IF (opt = 1) THEN
        option$ = _
"      >>>  EXTENDED LIBRARY vs. STANDARD LIBRARY, NO IONS PERMITTED  <<<"
        READ file1.sum$, file2.sum$
        READ file1.out$, file2.out$
        out.ext$ = ".1"

    ELSEIF (opt = 2) THEN
        option$ = _
"       >>>  EXTENDED LIBRARY vs. STANDARD LIBRARY, IONS PERMITTED  <<<"
        FOR i = 1 TO 4: READ JUNK$: NEXT
        READ file1.sum$, file2.sum$
        READ file1.out$, file2.out$
        out.ext$ = ".2"
  ELSE
        option$ = _
"       >>>  EXTENDED LIBRARY: IONS EXCLUDED vs. IONS INCLUDED  <<<"
        FOR i = 1 TO 8: READ JUNK$: NEXT
        READ file1.sum$, file2.sum$
        READ file1.out$, file2.out$
        out.ext$ = ".3"

  END IF
```

```
file$ = "OUTPUT" + out.ext$
OPEN file$ FOR OUTPUT AS #9
file$ = "INTERMED" + out.ext$
OPEN file$ FOR OUTPUT AS #33
file$ = "BRIEF" + out.ext$
OPEN file$ FOR OUTPUT AS #253
' PRINT #9, "  Option chosen."
PRINT #9, option$

PRINT #9,
PRINT #9, _
"       The two EXMUCET output files are "; file1.out$; " and "; file2.out$
PRINT #9,
GOSUB lib.name: ' Try to determine which library was used

PRINT #9, _
"       The input (SUMMARY) files are "; file1.sum$; " and "; file2.sum$
PRINT #9,



PRINT #253, : PRINT #253, "  First EXMUCET output file  = "; file1.out$
PRINT #253, "  Second EXMUCET output file = "; file2.out$: PRINT #253,
PRINT #253, "  Input (SUMMARY) files are "; file1.sum$; " and "
PRINT #253, "                            "; file2.sum$: ' PRINT #253,

'PRINT "  Input (OUTPUT) files are "; file1.out$; " and "
'PRINT "                           "; file2.out$: PRINT " "

PRINT #9, "  Thermo library used for first set was "
PRINT #9, TAB(19); lib.name.1$: PRINT #9, " "
PRINT #9, "  Thermo library used for second set was "
PRINT #9, TAB(19); lib.name.2$

' Initialization for first file
OPEN file1.sum$ FOR INPUT AS #1
OPEN "TEMPO1" FOR OUTPUT AS #2
LINE.NO = 0: LK = 0: kase = 0: num.of.energies = 0

' Read a line of first input file
READ1: LINE INPUT #1, lyne$

        IF (EOF(1)) THEN GOTO NEXT.FILE
        IF (LEFT$(lyne$, 5) = " Finis") THEN
            PRINT CHR$(7); CHR$(7); CHR$(7)
            GOTO NEXT.FILE
        END IF
```

```
' Look for sentinel ('>')
CONTTX:      IF (LEFT$(lyne$, 2) <> " >") THEN GOTO READ1

' Sentinel has been found. Increment case counter.
    kase = kase + 1
    GOSUB get.energy

'Next, skip 3 lines
LINE INPUT #1, JUNK1$: LINE INPUT #1, JUNK2$: LINE INPUT #1, JUNK3$
' Read line of data, and extract temperature, impetus, and ballergy
LINE INPUT #1, lyne$
    temp1(kase) = VAL(MID$(lyne$, 25, 9))
    gmptus1(kase) = VAL(MID$(lyne$, 49, 8))
    ballergy1(kase) = VAL(MID$(lyne$, 63, 8))
' PRINT "1 "; kase; num.kase1(kase); temp1(kase); gmptus1(kase); _
ballergy1(kase)
    PRINT #2, num.kase1(kase); ","; temp1(kase); ","; gmptus1(kase); ","; _
                                                    ballergy1(kase)
    GOTO READ1

' When end of-of-file has been found, write sentinel at end and close files
NEXT.FILE:  num.nrgy = kase: ' PRINT "LAST KASE ="; num.nrgy
  PRINT #2, "-9999., -9999., -9999.": PRINT #2, " ": CLOSE #1: CLOSE #2

' Initialization for second file
OPEN file2.sum$ FOR INPUT AS #1
OPEN "TEMPO2" FOR OUTPUT AS #2

kase = 0
READ2:
LINE INPUT #1, lyne$:
' IF (EOF(1) OR LEFT$(LYNE$, 5) = " Finis") THEN GOTO MAKE.TAB

        IF (EOF(1)) GOTO MAKE.TAB
        IF (LEFT$(lyne$, 5) = " Finis") THEN
        PRINT CHR$(7); CHR$(7); CHR$(7)
        GOTO MAKE.TAB
        END IF

    IF (LEFT$(lyne$, 2) <> " >") THEN GOTO READ2
    kase = kase + 1
    num.kase2(kase) = kase
LINE INPUT #1, JUNK$: LINE INPUT #1, JUNK$: LINE INPUT #1, JUNK$
```

```
LINE INPUT #1, lyne$
     temp2(kase) = VAL(MID$(lyne$, 25, 9))
     gmptus2(kase) = VAL(MID$(lyne$, 49, 8))
     ballergy2(kase) = VAL(MID$(lyne$, 63, 7))
'PRINT "2 "; kase; num.kase2(kase); temp2(kase); gmptus2(kase); _
ballergy2(kase)
     PRINT #2, num.kase2(kase); ","; temp2(kase); ","; gmptus2(kase); ","; _
                                                  ballergy2(kase)
     GOTO READ2

MAKE.TAB:  PRINT #2, "-9999., -9999., -9999.": PRINT #2, " "
CLOSE #1: CLOSE #2
'                          PRINT "-9999., -9999., -9999."; num.nrgy
PRINT #9, : PRINT #9, " Number of energies = "; no.ener: ' PRINT

' Get ready to make summary table (previously-opened)
OPEN "tempo1" FOR INPUT AS #1
OPEN "tempo2" FOR INPUT AS #2
' PRINT "Run option chosen = "; run.option$
IF (opt <> 3) THEN

head3$ = _
"     T(Std)   T(Ext)  Imp(Std) Imp(Ext)  Ball(Std) Ball(Ext) Gam(Std) _
                                                    Gam(Ext)"
head33$ = _
"     T(Std)  T(Ext)  Delta T   %DelT   Ball(Std) Ball(Ext) DeltaB  %DelB"
   ELSE
head3$ = _
"     T(no)   T(ions)  Imp(no)  Imp(ion)  Ball(no) Ball(ion) Gam(no)_
                                                    Gam(ion)"
head33$ = _
"   T(no)   T(ions)  Delta T   %DelT   Ball(no) Ball(ion) Delta Ball %DelB"
   END IF

' Read a line of data from file 1
   FOR i = 1 TO 999
INPUT #1, num.kase1(i), temp1(i), gmptus1(i), ballergy1(i)
       IF (temp1(i) > 0) THEN GOTO NEXTT1 ELSE GOTO CONTT1
NEXTT1: NEXT
CONTT1: num.1 = i - 1

' Read a line of input from file 2
FOR i = 1 TO 999: INPUT #2, num.kase2(i), temp2(i), gmptus2(i), ballergy2(i)
       IF (temp2(i) > 0) THEN GOTO NEXTT2 ELSE GOTO CONTT2
NEXTT2: NEXT
CONTT2: NUM.2 = i - 1
```

```
' Check that same number of lines have been read
IF (num.1 = NUM.2 AND num.kase1(num.nrgy) = num.kase2(num.nrgy)) _
THEN GOTO NEXTT3
CLS : PRINT "T R O U B L E !!!  NUM.1 <> NUM.2"; NUM.1;NUM2. : STOP

NEXTT3:
' Print summary table with statistics after each group

FOR i.ener = 1 TO no.ener:

        PRINT #9, : PRINT #9, TAB(30); e.zero(i.ener); "kJ/g added"
        PRINT #253, : PRINT #253, TAB(25); e.zero(i.ener); "kJ/g added"
        PRINT #33, : PRINT #33, TAB(30); e.zero(i.ener); "kJ/g added"
        PRINT #33, head33$
        PRINT #9, head3$

'     FOR jj = no.cmpsns * i.ener - (no.cmpsns - 1) TO no.cmpsns * i.ener
      FOR jj = no.cmpsns * (i.ener - 1) + 1 TO no.cmpsns * i.ener
      num.case = jj MOD no.cmpsns: IF num.case = 0 THEN num.case = no.cmpsns

PRINT #9, USING _
" ##) ######.# ######.# ######.# ######.#  ######.# ######.#  ##.#### _
  ##.####"; num.case; temp1(jj); temp2(jj); gmptus1(jj); gmptus2(jj); _
     ballergy1(jj); ballergy2(jj); 1! + gmptus1(jj) / ballergy1(jj); _
                                   1! + gmptus2(jj) / ballergy2(jj)

PRINT #33, USING _
"##) ######.# ######.# #####.# ##.####  ######.# ######.# ######.# ##.##";_
                num.case; temp1(jj); temp2(jj); temp2(jj) - temp1(jj); _
            100! * (temp2(jj) - temp1(jj)) / temp1(jj); ballergy1(jj); _
                       ballergy2(jj); ballergy2(jj) - ballergy1(jj); _
                100! * (ballergy2(jj) - ballergy1(jj)) / ballergy1(jj)
      NEXT jj
      GOSUB STAT
NEXT i.ener

' Prepare and print table of differences

PRINT #33,

PRINT #9, :       PRINT #9, TAB(26); "G R A N D   T O T A L S": PRINT #9,
PRINT #9, TAB(26); "MEAN ABSOLUTE DEVIATIONS"
PRINT #9, TAB(13); "Temp (K)          Impetus (J/g)      Ballergy (J/g)"
```

```
PRINT #33, :  PRINT #33, TAB(26); "G R A N D   T O T A L S": PRINT #33,
PRINT #33, TAB(26); "MEAN ABSOLUTE DEVIATIONS"
PRINT #33, TAB(13); "Temp (K)          Impetus (J/g)      Ballergy (J/g)"

sum.t1 = 0!: sum.t2 = 0!: sum.t3 = 0!: sum.t4 = 0!
sum.g1 = 0!: sum.g2 = 0!: sum.g3 = 0!: sum.g4 = 0!
sum.b1 = 0!: sum.b2 = 0!: sum.b3 = 0!: sum.b4 = 0!

FOR i = 1 TO num.1
Delta.t(i) = temp2(i) - temp1(i): Delta.g(i) = gmptus2(i) - gmptus1(i)
Delta.b(i) = ballergy2(i) - ballergy1(i): NEXT i

FOR i = 1 TO num.1
      sum.t1 = sum.t1 + ABS(Delta.t(i)):
      sum.g1 = sum.g1 + ABS(Delta.g(i)):
      sum.b1 = sum.b1 + ABS(Delta.b(i)):
      sum.t2 = sum.t2 + ABS(Delta.t(i)) / temp1(i)
      sum.g2 = sum.g2 + ABS(Delta.g(i)) / gmptus1(i)
      sum.b2 = sum.b2 + ABS(Delta.b(i)) / ballergy1(i)
      sum.t3 = sum.t3 + Delta.t(i) ^ 2
      sum.g3 = sum.g3 + Delta.g(i) ^ 2
      sum.b3 = sum.b3 + Delta.b(i) ^ 2
      sum.t4 = sum.t4 + (Delta.t(i) / temp1(i)) ^ 2
      sum.g4 = sum.g4 + (Delta.g(i) / gmptus1(i)) ^ 2
      sum.b4 = sum.b4 + (Delta.b(i) / ballergy1(i)) ^ 2
NEXT i

PRINT #9, _
USING "          ###.#            ###.#            ######.#    "; _
      sum.t1 / (num.1 - 1); sum.g1 / (num.1 - 1); sum.b1 / (num.1 - 1)
PRINT #9, :            PRINT #9, TAB(21); "MEAN ABSOLUTE PERCENT DEVIATIONS"
PRINT #9, TAB(14); "Temp (K)       Impetus (J/g)      Ballergy (J/g)"
 PRINT #9, USING _
         "           #.###            #.##            ####.##  "; _
            100 * sum.t2 / (num.1 - 1); 100 * sum.g2 / (num.1 - 1); _
                                        100 * sum.b2 / (num.1 - 1)
PRINT #9, :            PRINT #9, TAB(23); "ROOT MEAN SQUARE DEVIATIONS"
 PRINT #9, TAB(13); "Temp (K)          Impetus (J/g)      Ballergy (J/g)"
 PRINT #9, USING _
         "           ###.#            ###.#            ######.#    "; _
              SQR(sum.t3 / (num.1 - 1)); SQR(sum.g3 / (num.1 - 1)); _
                                         SQR(sum.b3 / (num.1 - 1))
PRINT #9, : PRINT #9, TAB(20); "ROOT MEAN SQUARE PERCENT DEVIATIONS"
PRINT #9, TAB(13); "Temp (K)          Impetus (J/g)      Ballergy (J/g)"
PRINT #9, USING _
        "           ##.##            ##.##            #####.#    "; _
     100 * SQR(sum.t4 / (num.1 - 1)); 100 * SQR(sum.g4 / (num.1 - 1)); _
                                      100 * SQR(sum.b4 / (num.1 - 1))
```

```
PRINT #33, _
USING "          ###.#          ###.#          #####.#    "; _
        sum.t1 / (num.1 - 1); sum.g1 / (num.1 - 1); sum.b1 / (num.1 - 1)
PRINT #33, : PRINT #33, TAB(21); "MEAN ABSOLUTE PERCENT DEVIATIONS"
PRINT #33, TAB(14); "Temp (K)       Impetus (J/g)      Ballergy (J/g)"

   PRINT #33, USING _
          "          #.###          #.##          ####.##  "; _
              100 * sum.t2 / (num.1 - 1); 100 * sum.g2 / (num.1 - 1); _
                                  100 * sum.b2 / (num.1 - 1)
PRINT #33, :          PRINT #33, TAB(23); "ROOT MEAN SQUARE DEVIATIONS"
PRINT #33, TAB(13); "Temp (K)       Impetus (J/g)      Ballergy (J/g)"

 PRINT #33, USING _
      "          ###.#          ###.#          #####.#    "; _
             SQR(sum.t3 / (num.1 - 1)); SQR(sum.g3 / (num.1 - 1)); _
SQR(sum.b3 / (num.1 - 1))
PRINT #33, : PRINT #33, TAB(20); "ROOT MEAN SQUARE PERCENT DEVIATIONS"
PRINT #33, TAB(13); "Temp (K)       Impetus (J/g)      Ballergy (J/g)"
PRINT #33, _
    USING "          ##.##          ##.##          ####.#    "; _
       100 * SQR(sum.t4 / (num.1 - 1)); 100 * SQR(sum.g4 / (num.1 - 1)); _
                                  100 * SQR(sum.b4 / (num.1 - 1))

PRINT #33, : PRINT #33, : PRINT #33,
PRINT #253, : PRINT #253, : PRINT #253,

COLOR 15, 0
CLOSE #1: CLOSE #2: CLOSE #33
KILL "TEMPO1": KILL "TEMPO2"
SYSTEM

get.energy: FOR J = 3 TO LEN(lyne$): SENT$ = MID$(lyne$, J, 1)
   IF (SENT$ <> " ") THEN GOTO CONTT3
NEXT: PRINT " T R O U B L E   in Subroutine GET.ENERGY.  LYNE$ = "; lyne$
STOP

CONTT3: llen = LEN(lyne$)
      FOR ll = llen TO 1 STEP -1
        IF (MID$(lyne$, ll, 1) = "J") THEN GOTO contt4
      NEXT ll
contt4: IF (MID$(lyne$, ll - 1, 4) = "kJ/g") THEN GOTO contt5
       CLS : PRINT "RATS! Problem at "; CHR$(34); " contt4"; CHR$(34): STOP
contt5: ll.j = ll
      FOR ll = ll.j TO 1 STEP -1
      IF (MID$(lyne$, ll, 1) = "+") THEN GOTO contt6
      NEXT ll
        PRINT "RATS! Problem at "; CHR$(34); " contt5"; CHR$(34): STOP
```

```
cont6: energy = VAL(MID$(lyne$, ll + 1, ll.j - ll + 1))
'                              PRINT "Energy = "; energy
        IF (energy = energy.save) THEN GOTO returnn
        energy.save = energy
        no.ener = no.ener + 1
        e.zero(no.ener) = energy
'                                  print "Energy = "; energy
returnn: RETURN

STAT.SUM:
  FOR jj = 1 TO no.ener: ii = jj + no.cmpns * (i.ener - 1)
      sum.t1 = sum.t1 + ABS(Delta.t(ii))
      sum.t2 = sum.t2 + ABS(Delta.t(ii)) / temp1(ii)
      sum.g1 = sum.g1 + ABS(Delta.g(ii))
      sum.g2 = sum.g2 + ABS(Delta.g(ii)) / gmptus1(ii)
      sum.b1 = sum.b1 + ABS(Delta.b(ii))
      sum.b2 = sum.b2 + ABS(Delta.b(ii)) / ballergy1(ii)
NEXT jj

'    PRINT USING _
"            #.###              #.###            ##.###  "; _
          100 * sum.t2 / num.1; 100 * sum.g2 / num.1; 100 * sum.b2 / num.1

RETURN

' A subroutine that tries to determine which thermo library was used
lib.name:
OPEN file1.out$ FOR INPUT AS #2:
reads1: LINE INPUT #2, lyne$
      IF (LEFT$(lyne$, 40) = " SPECIES BEING CONSIDERED IN THIS SYSTEM") THEN
        lib.name.1$ = "McBride's standard (CET89) library"
        GOTO close2
      END IF
    FOR jk = 1 TO LEN(lyne$)
      IF (MID$(lyne$, jk, 3) <> "***") THEN GOTO nexxt1
      lib.name.1$ = RIGHT$(lyne$, 81 - jk): GOTO close2
nexxt1: NEXT: GOTO reads1
close2: CLOSE #2

OPEN file2.out$ FOR INPUT AS #2
reads3: LINE INPUT #2, lyne$
      IF (LEFT$(lyne$, 40) = "SPECIES BEING CONSIDERED IN THIS SYSTEM") THEN
        lib.name.2$ = "McBride's standard (CET89) library"
        GOTO close2a
      END IF
    FOR jk = 1 TO LEN(lyne$)
        IF (MID$(lyne$, jk, 3) <> "***") THEN GOTO nexxt2
        lib.name.2$ = RIGHT$(lyne$, 81 - jk): GOTO close2a
nexxt2: NEXT: GOTO reads3
```

```
close2a: CLOSE #2: RETURN

' Check prints
' CLS : PRINT file1.out$, file2.out$
' PRINT line.counter.1, line.counter.2
' PRINT lib.name.1$; " and "; lib.name.2$

CLOSE #2
RETURN

' A subroutine that computes statistics for each energy

STAT:

    sum.t1 = 0!: sum.t2 = 0!: sum.g1 = 0!
    sum.g2 = 0!: i.max.b = 1: i.max.t = 1
    sum.b1 = 0!: sum.b2 = 0!: d.pct.ball.max = 0: d.pct.temp.max = 0

 FOR nki = 1 TO no.cmpsns: ii = nki + no.cmpsns * (i.ener - 1)

    Delta.g(ii) = gmptus2(ii) - gmptus1(ii)
  Delta.pct.t(ii) = (temp2(ii) - temp1(ii)) / temp1(ii)
  Delta.pct.b(ii) = (ballergy2(ii) - ballergy1(ii)) / ballergy1(ii)
    IF (ABS(Delta.pct.b(ii)) > d.pct.ball.max) THEN
      d.pct.ball.max = ABS(Delta.pct.b(ii)): i.max.b = nki
      d.ball.max = ballergy2(ii) - ballergy1(ii)
    END IF
    IF (ABS(Delta.pct.t(ii)) > d.pct.temp.max) THEN
      d.pct.temp.max = ABS(Delta.pct.t(ii)): i.max.t = nki
      temp.max = temp1(ii)
    END IF
  NEXT nki

PRINT #9, TAB(13);
IF (100! * d.pct.temp.max >= .1) THEN
 PRINT #9, USING _
"Max abs pct diff in TEMPERATURE = ##.#% for case no. ##"; _
                                  100! * d.pct.temp.max; i.max.t
ELSE
PRINT #9, USING _
         "Max abs pct diff in TEMPERATURE = #.##% for case no. ##"; _
                                  100! * d.pct.temp.max; i.max.t
END IF
PRINT #33, TAB(13);
PRINT #33, USING "Max abs pct diff in TEMPERATURE = ##.#% for case no. ##"; _
                                  100! * d.pct.temp.max; i.max.t
```

```
PRINT #253, TAB(3);
PRINT #253, USING "Max abs pct diff in TEMPERATURE = ##.#% for case no. ##"; _
                                  100! * d.pct.temp.max; i.max.t

PRINT #9, TAB(13);
IF (100! * d.pct.ball.max >= .1) THEN
  PRINT #9, USING "Max abs pct diff in BALLERGY    = ##.#% for case no. ##"; _
                                  100! * d.pct.ball.max; i.max.b
ELSE
  PRINT #9, USING "Max abs pct diff in BALLERGY    = #.##% for case no. ##"; _
                                  100! * d.pct.ball.max; i.max.b
END IF
PRINT #253, TAB(3);
PRINT #253, USING "Max abs pct diff in BALLERGY    = ##.#% for case no. ##"; _
                                  100! * d.pct.ball.max; i.max.b

PRINT #33, TAB(13);
PRINT #33, USING "Max abs pct diff in BALLERGY    = ##.#% for case no. ##"; _
                                  100! * d.pct.ball.max; i.max.b

' PRINT TAB(24); "Mean Absolute Deviations"
' PRINT TAB(14); "Temp              Impetus          Ballergy"

  RETURN:  ' end of STAT

DATA "d:\exmuce\TSTLBSNO.STD" : '  Summary table, no ions, standard library
DATA "d:\exmuce\TSTLBSNO.EXT" : '  Summary table, no ions, extended library
DATA "d:\exmuce\TSTLBONO.STD" : '  Output table,  no ions, standard library
DATA "d:\exmuce\TSTLBONO.EXT" : '  Output table,  no ions, extended library

DATA "d:\exmuce\TSTLBSIO.STD" : '  Summary table, w/ ions, standard library
DATA "d:\exmuce\TSTLBSIO.EXT" : '  Summary table, w/ ions, extended library
DATA "d:\exmuce\TSTLBOIO.STD" : '  Output table,  w/ ions, standard library
DATA "d:\exmuce\TSTLBOIO.EXT" : '  Output table,  w/ ions, extended library

DATA "d:\exmuce\TSTLBSNO.EXT" : '  Summary table, no ions, extended library
DATA "d:\exmuce\TSTLBSIO.EXT" : '  Summary table, w/ ions, extended library
DATA "d:\exmuce\TSTLBONO.EXT" : '  Output table,  no ions, extended library
DATA "d:\exmuce\TSTLBOIO.EXT" : '  Output table,  w/ ions, extended library
```

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Appendix E.

Output from COMPARE.BAS:
Comparing the Results from the Standard (CET89) Library with
Those from McBride's Extended Library—Ions Excluded

The two EXMUCET output files are TSTLBONO.STD and TSTLBONO.EXT

The input (SUMMARY) files are TSTLBSNO.STD and TSTLBSNO.EXT

Thermo library used for first set was
*** McBride's Standard (CET89) Library ***

Thermo library used for second set was
*** B. McBride's EXTENDED-RANGE Library ***

Number of energies = 21

0 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3017.2	3010.2	1080.6	1077.9	4563.5	4583.2	1.2368	1.2352
2)	2552.1	2549.1	944.8	943.5	3729.1	3736.5	1.2534	1.2525
3)	3401.5	3392.2	1139.7	1136.3	5157.6	5184.0	1.2210	1.2192
4)	3820.8	3811.9	1176.9	1173.5	5686.2	5723.1	1.2070	1.2050
5)	2492.9	2490.6	929.0	927.9	3583.1	3588.6	1.2593	1.2586
6)	3748.7	3738.6	1202.4	1198.2	6217.5	6278.9	1.1934	1.1908
7)	1220.6	1216.5	474.6	472.6	2870.8	2899.8	1.1653	1.1630
8)	3588.9	3574.6	1388.7	1382.5	6534.2	6590.0	1.2125	1.2098

Max abs pct diff in TEMPERATURE = 0.4% for case no. 8
Max abs pct diff in BALLERGY = 1.0% for case no. 7

.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3320.1	3311.4	1191.1	1187.7	5074.8	5099.6	1.2347	1.2329
2)	2881.3	2877.0	1067.5	1065.7	4274.3	4285.1	1.2497	1.2487
3)	3674.1	3664.1	1235.8	1232.0	5609.1	5640.6	1.2203	1.2184
4)	4022.5	4014.0	1251.2	1247.7	5996.8	6038.1	1.2086	1.2066
5)	2828.0	2824.6	1054.8	1053.3	4129.1	4137.5	1.2555	1.2546
6)	3903.8	3893.8	1266.6	1262.1	6479.5	6545.9	1.1955	1.1928
7)	1306.9	1302.5	534.0	531.7	3121.9	3155.1	1.1710	1.1685
8)	3795.4	3781.1	1475.7	1469.2	6948.8	7012.6	1.2124	1.2095

Max abs pct diff in TEMPERATURE = 0.4% for case no. 8
Max abs pct diff in BALLERGY = 1.1% for case no. 7

1 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3601.2	3591.6	1295.7	1291.9	5549.3	5578.8	1.2335	1.2316
2)	3198.8	3193.1	1186.4	1184.1	4801.2	4816.0	1.2471	1.2459
3)	3919.4	3909.3	1325.7	1321.7	6013.0	6049.3	1.2205	1.2185
4)	4203.7	4195.5	1322.5	1318.7	6270.2	6315.7	1.2109	1.2088
5)	3152.5	3147.7	1177.0	1175.0	4659.2	4671.3	1.2526	1.2515
6)	4050.1	4040.1	1330.1	1325.3	6723.2	6794.5	1.1978	1.1951
7)	1392.1	1387.5	597.5	594.8	3364.9	3400.3	1.1776	1.1749
8)	3983.1	3969.3	1558.2	1551.5	7323.1	7395.0	1.2128	1.2098

Max abs pct diff in TEMPERATURE = 0.3% for case no. 8
Max abs pct diff in BALLERGY = 1.1% for case no. 6

1.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3858.0	3848.1	1394.2	1390.1	5981.7	6015.6	1.2331	1.2311
2)	3500.2	3493.2	1300.6	1297.8	5302.5	5321.0	1.2453	1.2439
3)	4139.4	4129.7	1410.5	1406.3	6371.8	6413.0	1.2214	1.2193
4)	4371.0	4363.1	1392.1	1388.1	6517.5	6567.7	1.2136	1.2114
5)	3461.6	3455.7	1294.6	1292.2	5165.8	5181.3	1.2506	1.2494
6)	4190.1	4180.2	1393.4	1388.3	6953.6	7029.8	1.2004	1.1975
7)	1478.4	1473.6	665.6	662.5	3606.6	3642.4	1.1846	1.1819
8)	4154.9	4141.9	1637.2	1630.4	7663.0	7743.0	1.2136	1.2106

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.1% for case no. 6

2 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4090.8	4081.4	1487.1	1482.8	6372.1	6410.5	1.2334	1.2313
2)	3782.2	3774.5	1409.7	1406.5	5773.0	5794.3	1.2442	1.2427
3)	4338.5	4329.4	1491.4	1487.0	6692.3	6738.9	1.2229	1.2207
4)	4528.8	4521.1	1461.1	1457.0	6746.4	6802.2	1.2166	1.2142
5)	3752.1	3745.4	1407.1	1404.3	5643.6	5661.6	1.2493	1.2480
6)	4325.3	4315.5	1456.9	1451.5	7173.7	7255.3	1.2031	1.2001
7)	1567.4	1562.4	738.6	735.3	3851.5	3886.6	1.1918	1.1892
8)	4313.8	4301.6	1713.7	1706.7	7974.7	8062.8	1.2149	1.2117

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.1% for case no. 6

2.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4302.8	4294.0	1575.5	1571.2	6724.7	6768.2	1.2343	1.2321
2)	4043.6	4035.6	1513.5	1510.0	6209.5	6233.5	1.2437	1.2422
3)	4521.3	4512.9	1569.8	1565.2	6982.0	7035.1	1.2248	1.2225
4)	4680.1	4672.8	1530.3	1525.9	6961.9	7024.8	1.2198	1.2172
5)	4022.4	4015.3	1514.3	1511.2	6089.2	6109.3	1.2487	1.2474
6)	4456.9	4447.4	1520.9	1515.2	7385.9	7473.5	1.2059	1.2027
7)	1660.3	1655.4	817.0	813.3	4103.8	4137.5	1.1991	1.1966
8)	4462.4	4451.2	1788.4	1781.3	8263.7	8360.1	1.2164	1.2131

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.2% for case no. 6

3 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4497.7	4489.8	1660.6	1656.2	7045.6	7095.0	1.2357	1.2334
2)	4285.0	4277.2	1612.7	1609.0	6611.9	6638.8	1.2439	1.2424
3)	4692.1	4684.3	1646.6	1641.9	7247.9	7308.8	1.2272	1.2246
4)	4827.1	4820.0	1599.9	1595.4	7167.2	7239.3	1.2232	1.2204
5)	4272.9	4265.9	1616.8	1613.6	6502.0	6524.3	1.2487	1.2473
6)	4585.8	4576.4	1585.6	1579.6	7591.5	7686.1	1.2089	1.2055
7)	1758.8	1754.0	900.8	897.0	4368.4	4400.1	1.2062	1.2039
8)	4603.1	4592.7	1862.1	1854.9	8534.5	8639.8	1.2182	1.2147

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.2% for case no. 6

3.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4679.2	4672.3	1743.4	1739.1	7340.6	7397.4	1.2375	1.2351
2)	4508.4	4501.0	1707.9	1704.1	6982.0	7013.1	1.2446	1.2430
3)	4853.8	4846.7	1722.7	1717.9	7494.9	7565.8	1.2298	1.2271
4)	4971.0	4964.2	1670.5	1665.7	7364.5	7448.1	1.2268	1.2236
5)	4505.2	4498.6	1715.3	1711.9	6883.2	6908.8	1.2492	1.2478
6)	4712.5	4703.3	1651.0	1644.8	7791.7	7894.3	1.2119	1.2084
7)	1864.4	1859.8	990.3	986.4	4650.8	4680.3	1.2129	1.2108
8)	4737.3	4727.8	1935.2	1927.9	8790.6	8905.3	1.2201	1.2165

Max abs pct diff in TEMPERATURE = 0.2% for case no. 7
Max abs pct diff in BALLERGY = 1.3% for case no. 6

4 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4850.5	4844.6	1824.9	1820.6	7614.5	7681.0	1.2397	1.2370
2)	4716.4	4709.6	1800.1	1796.3	7322.8	7360.3	1.2458	1.2441
3)	5009.0	5002.4	1798.8	1793.8	7726.9	7810.4	1.2328	1.2297
4)	5113.0	5106.4	1742.1	1737.1	7554.9	7653.2	1.2306	1.2270
5)	4721.9	4715.9	1810.6	1807.2	7235.2	7266.4	1.2502	1.2487
6)	4837.4	4828.6	1717.4	1710.9	7987.2	8099.2	1.2150	1.2112
7)	1978.7	1974.5	1085.2	1081.3	4957.0	4984.6	1.2189	1.2169
8)	4866.5	4857.9	2008.0	2000.6	9034.6	9159.6	1.2223	1.2184

Max abs pct diff in TEMPERATURE = 0.2% for case no. 7
Max abs pct diff in BALLERGY = 1.4% for case no. 6

4.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5014.0	5008.9	1905.8	1901.4	7871.0	7949.9	1.2421	1.2392
2)	4911.6	4905.5	1890.2	1886.4	7637.8	7684.6	1.2475	1.2455
3)	5159.3	5153.3	1875.1	1870.0	7946.4	8045.7	1.2360	1.2324
4)	5253.7	5247.4	1815.0	1809.7	7739.0	7855.8	1.2345	1.2304
5)	4925.4	4920.0	1903.5	1900.1	7560.7	7600.9	1.2518	1.2500
6)	4961.0	4952.5	1784.9	1778.1	8178.4	8301.4	1.2182	1.2142
7)	2102.4	2099.0	1184.9	1181.3	5291.1	5318.0	1.2239	1.2221
8)	4991.6	4983.8	2080.9	2073.4	9268.4	9404.8	1.2245	1.2205

Max abs pct diff in TEMPERATURE = 0.2% for case no. 6
Max abs pct diff in BALLERGY = 1.5% for case no. 4

5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5171.6	5167.3	1986.4	1982.1	8112.8	8207.6	1.2448	1.2415
2)	5096.5	5091.1	1978.9	1975.0	7929.8	7990.0	1.2496	1.2472
3)	5306.2	5300.6	1952.1	1946.8	8155.0	8274.1	1.2394	1.2353
4)	5393.7	5387.6	1889.3	1883.7	7916.9	8056.8	1.2386	1.2338
5)	5118.3	5113.5	1994.9	1991.5	7862.4	7916.1	1.2537	1.2516
6)	5083.5	5075.3	1853.4	1846.3	8365.6	8501.4	1.2216	1.2172
7)	2234.5	2232.7	1287.8	1284.9	5651.9	5680.7	1.2279	1.2262
8)	5113.5	5106.4	2154.1	2146.5	9493.5	9642.4	1.2269	1.2226

Max abs pct diff in TEMPERATURE = 0.2% for case no. 6
Max abs pct diff in BALLERGY = 1.8% for case no. 4

5.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5324.7	5321.1	2067.4	2063.0	8341.5	8456.6	1.2478	1.2440
2)	5273.3	5268.5	2066.8	2062.8	8201.5	8280.0	1.2520	1.2491
3)	5450.5	5445.2	2030.0	2024.4	8353.6	8497.3	1.2430	1.2382
4)	5533.5	5527.4	1965.1	1959.1	8088.4	8256.8	1.2430	1.2373
5)	5302.6	5298.3	2085.3	2081.8	8142.4	8215.5	1.2561	1.2534
6)	5205.1	5197.2	1923.0	1915.7	8548.9	8699.7	1.2249	1.2202
7)	2371.8	2372.8	1391.8	1390.3	6029.4	6064.7	1.2308	1.2292
8)	5232.7	5226.2	2227.8	2220.0	9710.9	9873.8	1.2294	1.2248

Max abs pct diff in TEMPERATURE = 0.2% for case no. 6
Max abs pct diff in BALLERGY = 2.1% for case no. 4

6 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5474.4	5471.3	2148.8	2144.3	8558.1	8698.6	1.2511	1.2465
2)	5443.7	5439.3	2154.4	2150.2	8454.5	8557.6	1.2548	1.2513
3)	5593.1	5588.0	2109.0	2103.1	8542.7	8716.4	1.2469	1.2413
4)	5673.3	5667.2	2042.5	2036.1	8252.8	8456.3	1.2475	1.2408
5)	5480.2	5476.2	2175.4	2171.7	8402.3	8502.0	1.2589	1.2554
6)	5326.1	5318.5	1993.9	1986.2	8728.3	8896.4	1.2284	1.2233
7)	2510.3	2515.2	1495.7	1495.9	6410.6	6456.5	1.2333	1.2317
8)	5349.6	5343.9	2302.0	2294.1	9921.4	10099.8	1.2320	1.2271

Max abs pct diff in TEMPERATURE = 0.2% for case no. 7
Max abs pct diff in BALLERGY = 2.5% for case no. 4

6.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5621.6	5618.8	2231.0	2226.3	8763.0	8935.3	1.2546	1.2492
2)	5609.2	5605.0	2242.1	2237.7	8690.0	8825.1	1.2580	1.2536
3)	5734.6	5729.6	2189.2	2182.9	8722.1	8932.6	1.2510	1.2444
4)	5813.6	5807.2	2121.6	2114.6	8409.3	8655.7	1.2523	1.2443
5)	5652.6	5648.7	2265.5	2261.4	8642.8	8778.0	1.2621	1.2576
6)	5446.6	5439.4	2066.0	2058.0	8903.7	9091.8	1.2320	1.2264
7)	2648.4	2657.2	1599.3	1601.0	6789.0	6846.4	1.2356	1.2338
8)	5464.8	5459.7	2376.9	2368.8	10125.5	10321.1	1.2347	1.2295

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 2.9% for case no. 4

7 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5767.0	5764.4	2314.1	2309.1	8955.9	9167.5	1.2584	1.2519
2)	5771.0	5766.8	2330.3	2325.5	8908.2	9084.4	1.2616	1.2560
3)	5875.5	5870.3	2270.9	2264.0	8891.1	9146.3	1.2554	1.2475
4)	5954.5	5947.7	2202.5	2194.8	8556.4	8855.2	1.2574	1.2479
5)	5821.0	5816.9	2355.9	2351.4	8863.8	9045.3	1.2658	1.2600
6)	5566.8	5559.8	2139.4	2131.0	9074.8	9286.0	1.2358	1.2295
7)	2786.6	2798.7	1703.3	1706.3	7166.0	7233.1	1.2377	1.2359
8)	5578.6	5574.0	2452.6	2444.4	10323.6	10538.4	1.2376	1.2320

Max abs pct diff in TEMPERATURE = 0.4% for case no. 7
Max abs pct diff in BALLERGY = 3.5% for case no. 4

7.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5911.2	5908.4	2398.3	2392.8	9136.2	9396.1	1.2625	1.2547
2)	5930.1	5925.5	2419.3	2413.8	9108.9	9336.9	1.2656	1.2585
3)	6016.2	6010.5	2354.0	2346.4	9048.8	9358.2	1.2601	1.2507
4)	6096.3	6088.7	2285.2	2276.6	8692.6	9054.8	1.2629	1.2514
5)	5986.6	5981.7	2447.0	2441.7	9064.6	9305.7	1.2700	1.2624
6)	5686.8	5680.0	2214.2	2205.4	9241.3	9479.0	1.2396	1.2327
7)	2926.2	2940.7	1808.4	1812.4	7546.9	7620.6	1.2396	1.2378
8)	5691.1	5687.1	2529.1	2520.7	10515.8	10751.9	1.2405	1.2344

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 4.2% for case no. 4

8 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6054.5	6051.3	2483.7	2477.5	9302.9	9621.7	1.2670	1.2575
2)	6087.2	6081.8	2509.1	2502.8	9291.0	9584.0	1.2701	1.2611
3)	6157.0	6150.6	2438.7	2430.1	9193.9	9568.6	1.2653	1.2540
4)	6239.3	6230.5	2369.9	2360.1	8815.9	9254.8	1.2688	1.2550
5)	6150.0	6144.0	2538.9	2532.6	9243.8	9560.2	1.2747	1.2649
6)	5806.8	5800.1	2290.3	2281.1	9402.8	9671.0	1.2436	1.2359
7)	3068.3	3084.2	1914.9	1919.6	7936.2	8013.3	1.2413	1.2396
8)	5802.8	5799.1	2606.5	2597.9	10702.2	10962.1	1.2435	1.2370

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 5.0% for case no. 4

8.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6197.5	6193.4	2570.4	2563.3	9454.3	9844.8	1.2719	1.2604
2)	6243.1	6236.4	2600.1	2592.6	9452.8	9826.4	1.2751	1.2638
3)	6298.3	6290.7	2525.1	2515.4	9324.5	9777.7	1.2708	1.2573
4)	6383.6	6373.1	2456.5	2445.3	8923.6	9455.2	1.2753	1.2586
5)	6312.1	6304.2	2631.9	2624.1	9399.2	9809.8	1.2800	1.2675
6)	5926.9	5920.2	2367.9	2358.1	9558.7	9861.8	1.2477	1.2391
7)	3213.3	3229.8	2022.8	2027.8	8336.6	8414.3	1.2426	1.2410
8)	5913.7	5910.4	2685.0	2676.1	10882.7	11169.2	1.2467	1.2396

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 6.0% for case no. 4

9 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6340.4	6334.9	2658.5	2650.2	9588.5	10065.7	1.2773	1.2633
2)	6398.2	6389.6	2692.3	2683.3	9592.2	10065.0	1.2807	1.2666
3)	6440.4	6431.1	2613.2	2602.0	9438.4	9985.8	1.2769	1.2606
4)	6529.4	6516.7	2545.3	2532.2	9012.9	9656.0	1.2824	1.2622
5)	6473.4	6462.8	2726.0	2716.3	9527.6	10055.4	1.2861	1.2701
6)	6047.1	6040.4	2447.0	2436.6	9708.4	10051.4	1.2520	1.2424
7)	3360.8	3377.3	2131.6	2136.8	8748.2	8824.7	1.2437	1.2421
8)	6024.0	6021.1	2764.4	2755.2	11057.1	11373.2	1.2500	1.2423

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 7.1% for case no. 4

9.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6483.5	6476.1	2748.1	2738.1	9703.1	10284.6	1.2832	1.2662
2)	6553.2	6541.8	2785.9	2774.8	9705.9	10300.2	1.2870	1.2694
3)	6583.4	6572.0	2703.2	2690.2	9532.8	10193.0	1.2836	1.2639
4)	6677.0	6661.3	2636.3	2620.8	9080.2	9857.2	1.2903	1.2659
5)	6634.3	6620.1	2821.5	2809.2	9625.3	10297.4	1.2931	1.2728
6)	6167.7	6160.8	2527.5	2516.5	9851.1	10239.9	1.2566	1.2458
7)	3510.0	3526.1	2240.8	2246.1	9169.4	9243.4	1.2444	1.2430
8)	6134.0	6131.3	2844.9	2835.3	11225.1	11574.3	1.2534	1.2450

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 8.6% for case no. 4

10 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6627.1	6617.0	2839.1	2827.2	9795.0	10501.7	1.2899	1.2692
2)	6708.2	6693.2	2881.0	2867.3	9790.4	10532.5	1.2943	1.2722
3)	6727.8	6713.3	2795.2	2779.7	9604.3	10399.3	1.2910	1.2673
4)	6826.7	6807.0	2729.6	2711.1	9121.1	10058.8	1.2993	1.2695
5)	6795.3	67[illegible]	2918.4	2902.8	9687.7	10536.4	1.3012	1.2755
6)	6288.7	62[illegible]	2609.6	2597.7	9985.9	10427.0	1.2613	1.2491
7)	3659.8	36[illegible]	2349.8	2355.0	9597.0	9667.9	1.2448	1.2436
8)	6243.7	6241.1	2926.5	2916.5	11386.3	11772.6	1.2570	1.2477

Max abs pct diff in TEMPERATURE = 0.4% for case no. 7
Max abs pct diff in BALLERGY = 10.3% for case no. 4

GRAND TOTALS

MEAN ABSOLUTE DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
7.5	6.0	177.0

MEAN ABSOLUTE PERCENT DEVIATIONS

Temp (K)	Impetus (J/g	Ballergy (J/g)
0.175	0.31	2.C1

ROOT MEAN SQUARE DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
8.3	6.7	262.1

ROOT MEAN SQUARE PERCENT DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
0.20	0.33	2.8

Appendix F.

Output from COMPARE.BAS:
Comparing the Results from the Standard (CET89) Library with Those from McBride's Extended Library—Ions Included

The two EXMUCET output files are TSTLBOIO.STD and TSTLBOIO.EXT

The input (SUMMARY) files are TSTLBSIO.STD and TSTLBSIO.EXT

Thermo library used for first set was
*** McBride's Standard (CET89) Library ***

Thermo library used for second set was
*** B. McBride's EXTENDED-RANGE Library ***

Number of energies = 21

0 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3017.2	3010.2	1080.6	1077.9	4563.5	4583.2	1.2368	1.2352
2)	2552.1	2549.1	944.8	943.5	3729.1	3736.5	1.2534	1.2525
3)	3401.5	3392.2	1139.7	1136.3	5157.6	5184.0	1.2210	1.2192
4)	3820.8	3811.9	1176.9	1173.5	5686.2	5723.1	1.2070	1.2050
5)	2492.9	2490.6	929.0	927.9	3583.1	3588.6	1.2593	1.2586
6)	3748.7	3738.6	1202.4	1198.2	6217.5	6278.9	1.1934	1.1908
7)	1220.6	1216.5	474.6	472.6	2870.8	2899.8	1.1653	1.1630
8)	3588.9	3574.6	1388.7	1382.5	6534.2	6590.1	1.2125	1.2098

Max abs pct diff in TEMPERATURE = 0.4% for case no. 8
Max abs pct diff in BALLERGY = 1.0% for case no. 7

.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3320.1	3311.4	1191.1	1187.7	5074.8	5099.6	1.2347	1.2329
2)	2881.3	2877.0	1067.5	1065.7	4274.3	4285.2	1.2497	1.2487
3)	3674.1	3664.1	1235.8	1232.0	5609.1	5640.6	1.2203	1.2184
4)	4022.5	4014.0	1251.2	1247.7	5996.8	6038.1	1.2086	1.2066
5)	2828.0	2824.6	1054.8	1053.3	4129.1	4137.6	1.2555	1.2546
6)	3903.8	3893.8	1266.6	1262.1	6479.5	6545.9	1.1955	1.1928
7)	1306.9	1302.5	534.0	531.7	3121.9	3155.1	1.1710	1.1685
8)	3795.4	3781.1	1475.7	1469.2	6948.8	7012.6	1.2124	1.2095

Max abs pct diff in TEMPERATURE = 0.4% for case no. 8
Max abs pct diff in BALLERGY = 1.1% for case no. 7

1 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3601.2	3591.6	1295.7	1291.9	5549.3	5578.8	1.2335	1.2316
2)	3198.8	3193.1	1186.4	1184.1	4801.2	4816.0	1.2471	1.2459
3)	3919.4	3909.3	1325.7	1321.7	6013.0	6049.3	1.2205	1.2185
4)	4203.7	4195.5	1322.4	1318.7	6270.2	6315.8	1.2109	1.2088
5)	3152.5	3147.7	1177.0	1175.0	4659.2	4671.3	1.2526	1.2515
6)	4050.1	4040.1	1330.1	1325.3	6723.2	6794.5	1.1978	1.1951
7)	1392.1	1387.5	597.5	594.8	3364.9	3400.3	1.1776	1.1749
8)	3983.1	3969.3	1558.2	1551.5	7323.1	7395.0	1.2128	1.2098

Max abs pct diff in TEMPERATURE = 0.3% for case no. 8
Max abs pct diff in BALLERGY = 1.1% for case no. 6

1.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	3858.0	3848.1	1394.2	1390.1	5981.7	6015.7	1.2331	1.2311
2)	3500.2	3493.2	1300.6	1297.8	5302.5	5321.0	1.2453	1.2439
3)	4139.4	4129.7	1410.5	1406.3	6371.8	6413.0	1.2214	1.2193
4)	4371.0	4363.1	1392.1	1388.1	6517.5	6567.7	1.2136	1.2114
5)	3461.6	3455.7	1294.6	1292.2	5165.8	5181.3	1.2506	1.2494
6)	4190.1	4180.2	1393.4	1388.3	6953.5	7029.8	1.2004	1.1975
7)	1478.4	1473.6	665.6	662.5	3606.6	3642.4	1.1846	1.1819
8)	4154.9	4141.9	1637.2	1630.4	7663.0	7743.0	1.2136	1.2106

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.1% for case no. 6

2 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4090.8	4081.4	1487.1	1482.8	6372.1	6410.6	1.2334	1.2313
2)	3782.2	3774.5	1409.7	1406.5	5773.0	5794.4	1.2442	1.2427
3)	4338.5	4329.4	1491.4	1487.0	6692.2	6738.9	1.2229	1.2207
4)	4528.8	4521.1	1461.1	1457.0	6746.4	6802.3	1.2166	1.2142
5)	3752.1	3745.4	1407.1	1404.3	5643.6	5661.6	1.2493	1.2480
6)	4325.3	4315.5	1456.9	1451.5	7173.7	7255.3	1.2031	1.2001
7)	1567.4	1562.4	738.6	735.3	3851.5	3886.6	1.1918	1.1892
8)	4313.8	4301.6	1713.7	1706.7	7974.7	8062.8	1.2149	1.2117

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.1% for case no. 6

2.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4302.8	4294.0	1575.5	1571.2	6724.7	6768.2	1.2343	1.2321
2)	4043.6	4035.6	1513.5	1510.0	6209.5	6233.5	1.2437	1.2422
3)	4521.3	4512.9	1569.8	1565.2	6982.0	7035.1	1.2248	1.2225
4)	4680.1	4672.8	1530.3	1525.9	6961.9	7024.8	1.2198	1.2172
5)	4022.4	4015.3	1514.3	1511.2	6089.2	6109.3	1.2487	1.2474
6)	4456.9	4447.4	1520.9	1515.2	7385.9	7473.5	1.2059	1.2027
7)	1660.3	1655.4	817.0	813.3	4103.8	4137.5	1.1991	1.1966
8)	4462.4	4451.2	1788.4	1781.3	8263.7	8360.1	1.2164	1.2131

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.2% for case no. 6

3 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4497.7	4489.8	1660.6	1656.2	7045.6	7095.0	1.2357	1.2334
2)	4285.0	4277.2	1612.7	1609.0	6611.8	6638.9	1.2439	1.2424
3)	4692.0	4684.3	1646.6	1641.9	7247.8	7308.8	1.2272	1.2246
4)	4827.0	4820.0	1599.9	1595.4	7167.2	7239.3	1.2232	1.2204
5)	4272.9	4265.9	1616.8	1613.6	6502.0	6524.3	1.2487	1.2473
6)	4585.8	4576.4	1585.6	1579.6	7591.5	7686.1	1.2089	1.2055
7)	1758.8	1754.0	900.8	897.0	4368.4	4400.1	1.2062	1.2039
8)	4603.0	4592.7	1862.1	1854.9	8534.5	8639.8	1.2182	1.2147

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 1.2% for case no. 6

3.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4679.2	4672.3	1743.4	1739.1	7340.5	7397.4	1.2375	1.2351
2)	4508.4	4501.0	1707.9	1704.1	6981.9	7013.1	1.2446	1.2430
3)	4853.8	4846.7	1722.7	1717.9	7494.9	7565.8	1.2298	1.2271
4)	4971.0	4964.2	1670.5	1665.7	7364.4	7448.1	1.2268	1.2236
5)	4505.2	4498.6	1715.3	1711.9	6883.2	6908.8	1.2492	1.2478
6)	4712.4	4703.3	1651.0	1644.8	7791.7	7894.3	1.2119	1.2084
7)	1864.4	1859.8	990.3	986.4	4650.8	4680.3	1.2129	1.2108
8)	4737.3	4727.8	1935.2	1927.9	8790.6	8905.3	1.2201	1.2165

Max abs pct diff in TEMPERATURE = 0.2% for case no. 7
Max abs pct diff in BALLERGY = 1.3% for case no. 6

4 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	4850.5	4844.6	1824.9	1820.6	7614.5	7680.9	1.2397	1.2370
2)	4716.3	4709.6	1800.1	1796.3	7322.8	7360.3	1.2458	1.2441
3)	5008.9	5002.4	1798.7	1793.8	7726.8	7810.4	1.2328	1.2297
4)	5112.9	5106.4	1742.1	1737.1	7554.8	7653.1	1.2306	1.2270
5)	4721.9	4715.9	1810.5	1807.2	7235.1	7266.4	1.2502	1.2487
6)	4837.4	4828.6	1717.4	1710.9	7987.2	8099.2	1.2150	1.2112
7)	1978.7	1974.5	1085.2	1081.3	4957.0	4984.6	1.2189	1.2169
8)	4866.5	4857.8	2008.0	2000.6	9034.6	9159.6	1.2223	1.2184

Max abs pct diff in TEMPERATURE = 0.2% for case no. 7
Max abs pct diff in BALLERGY = 1.4% for case no. 6

4.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5014.0	5008.9	1905.7	1901.4	7871.0	7949.9	1.2421	1.2392
2)	4911.5	4905.5	1890.2	1886.4	7637.7	7684.6	1.2475	1.2455
3)	5159.3	5153.3	1875.1	1870.0	7946.3	8045.7	1.2360	1.2324
4)	5253.6	5247.3	1814.9	1809.7	7738.9	7855.7	1.2345	1.2304
5)	4925.4	4920.0	1903.5	1900.1	7560.6	7600.8	1.2518	1.2500
6)	4960.9	4952.4	1784.8	1778.1	8178.3	8301.4	1.2182	1.2142
7)	2102.4	2099.0	1184.9	1181.3	5291.1	5318.0	1.2239	1.2221
8)	4991.6	4983.7	2080.9	2073.4	9268.4	9404.7	1.2245	1.2205

Max abs pct diff in TEMPERATURE = 0.2% for case no. 6
Max abs pct diff in BALLERGY = 1.5% for case no. 4

5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5171.6	5167.3	1986.4	1982.1	8112.7	8207.6	1.2449	1.2415
2)	5096.4	5091.1	1978.9	1975.0	7929.8	7990.0	1.2496	1.2472
3)	5306.1	5300.5	1952.1	1946.7	8154.9	8274.0	1.2394	1.2353
4)	5393.6	5387.5	1889.2	1883.6	7916.8	8056.6	1.2386	1.2338
5)	5118.2	5113.5	1994.9	1991.4	7862.3	7916.1	1.2537	1.2516
6)	5083.4	5075.2	1853.3	1846.3	8365.5	8501.4	1.2215	1.2172
7)	2234.5	2232.7	1287.8	1284.9	5651.9	5680.7	1.2279	1.2262
8)	5113.4	5106.3	2154.1	2146.5	9493.4	9642.4	1.2269	1.2226

Max abs pct diff in TEMPERATURE = 0.2% for case no. 6
Max abs pct diff in BALLERGY = 1.8% for case no. 4

5.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5324.6	5321.0	2067.3	2062.9	8341.4	8456.5	1.2478	1.2439
2)	5273.2	5268.4	2066.7	2062.8	8201.4	8280.0	1.2520	1.2491
3)	5450.4	5445.2	2030.0	2024.4	8353.5	8497.2	1.2430	1.2382
4)	5533.3	5527.3	1965.0	1959.1	8088.2	8256.6	1.2429	1.2373
5)	5302.5	5298.3	2085.3	2081.8	8142.3	8215.5	1.2561	1.2534
6)	5205.0	5197.2	1923.0	1915.6	8548.8	8699.6	1.2249	1.2202
7)	2371.8	2372.8	1391.8	1390.3	6029.4	6064.7	1.2308	1.2292
8)	5232.6	5226.2	2227.7	2220.0	9710.8	9873.7	1.2294	1.2248

Max abs pct diff in TEMPERATURE = 0.1% for case no. 6
Max abs pct diff in BALLERGY = 2.1% for case no. 4

6 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5474.3	5471.2	2148.8	2144.2	8558.0	8698.5	1.2511	1.2465
2)	5443.6	5439.2	2154.3	2150.2	8454.4	8557.5	1.2548	1.2513
3)	5593.0	5587.9	2108.9	2103.0	8542.5	8716.3	1.2469	1.2413
4)	5673.2	5667.1	2042.4	2036.0	8252.7	8456.2	1.2475	1.2408
5)	5480.1	5476.2	2175.3	2171.7	8402.2	8501.9	1.2589	1.2554
6)	5326.0	5318.5	1993.8	1986.2	8728.1	8896.3	1.2284	1.2233
7)	2510.3	2515.2	1495.7	1495.9	6410.6	6456.5	1.2333	1.2317
8)	5349.6	5343.8	2302.0	2294.1	9921.3	10099.6	1.2320	1.2271

Max abs pct diff in TEMPERATURE = 0.2% for case no. 7
Max abs pct diff in BALLERGY = 2.5% for case no. 4

6.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5621.5	5618.7	2230.9	2226.2	8762.8	8935.1	1.2546	1.2492
2)	5609.1	5605.0	2242.1	2237.7	8689.8	8825.0	1.2580	1.2536
3)	5734.5	5729.4	2189.2	2182.8	8721.9	8932.4	1.2510	1.2444
4)	5813.4	5807.1	2121.5	2114.5	8409.1	8655.5	1.2523	1.2443
5)	5652.4	5648.6	2265.4	2261.4	8642.6	8777.8	1.2621	1.2576
6)	5446.5	5439.3	2065.9	2057.9	8903.5	9091.6	1.2320	1.2264
7)	2648.4	2657.2	1599.3	1601.0	6789.0	6846.4	1.2356	1.2338
8)	5464.7	5459.6	2376.8	2368.8	10125.4	10320.9	1.2347	1.2295

Max abs pct diff in TEMPERATURE = 0.3% for case no. 7
Max abs pct diff in BALLERGY = 2.9% for case no. 4

7 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5766.9	5764.2	2314.0	2309.0	8955.7	9167.3	1.2584	1.2519
2)	5770.8	5766.7	2330.2	2325.4	8908.0	9084.2	1.2616	1.2560
3)	5875.3	5870.1	2270.7	2263.9	8890.8	9146.1	1.2554	1.2475
4)	5954.3	5947.5	2202.3	2194.7	8556.2	8854.9	1.2574	1.2479
5)	5820.8	5816.8	2355.8	2351.3	8863.6	9045.2	1.2658	1.2600
6)	5566.7	5559.7	2139.3	2131.0	9074.6	9285.8	1.2357	1.2295
7)	2786.6	2798.7	1703.3	1706.3	7166.0	7233.2	1.2377	1.2359
8)	5578.5	5573.9	2452.5	2444.3	10323.4	10538.1	1.2376	1.2319

Max abs pct diff in TEMPERATURE = 0.4% for case no. 7
Max abs pct diff in BALLERGY = 3.5% for case no. 4

7.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	5911.0	5908.2	2398.2	2392.7	9136.0	9395.8	1.2625	1.2547
2)	5929.8	5925.3	2419.1	2413.7	9108.6	9336.7	1.2656	1.2585
3)	6015.9	6010.3	2353.8	2346.3	9048.6	9357.9	1.2601	1.2507
4)	6096.0	6088.5	2285.0	2276.5	8692.3	9054.5	1.2629	1.2514
5)	5986.3	5981.6	2446.8	2441.6	9064.4	9305.4	1.2699	1.2624
6)	5686.7	5679.9	2214.1	2205.3	9241.1	9478.8	1.2396	1.2327
7)	2926.2	2940.7	1808.4	1812.4	7546.9	7620.6	1.2396	1.2378
8)	5691.0	5686.9	2529.0	2520.6	10515.6	10751.7	1.2405	1.2344

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 4.2% for case no. 4

8 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6054.3	6051.1	2483.6	2477.4	9302.6	9621.4	1.2670	1.2575
2)	6086.9	6081.6	2509.0	2502.7	9290.7	9583.7	1.2701	1.2611
3)	6156.7	6150.3	2438.5	2430.0	9193.6	9568.2	1.2652	1.2540
4)	6238.9	6230.2	2369.6	2359.9	8815.5	9254.4	1.2688	1.2550
5)	6149.7	6143.8	2538.7	2532.5	9243.5	9559.9	1.2746	1.2649
6)	5806.6	5799.9	2290.2	2281.0	9402.5	9670.6	1.2436	1.2359
7)	3068.3	3084.2	1914.9	1919.6	7936.2	8013.3	1.2413	1.2396
8)	5802.6	5799.0	2606.4	2597.8	10701.9	10961.8	1.2435	1.2370

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 5.0% for case no. 4

8.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6197.2	6193.1	2570.2	2563.2	9454.0	9844.4	1.2719	1.2604
2)	6242.7	6236.1	2599.9	2592.5	9452.5	9826.1	1.2750	1.2638
3)	6297.9	6290.4	2524.8	2515.2	9324.2	9777.2	1.2708	1.2573
4)	6383.1	6372.7	2456.2	2445.1	8923.3	9454.6	1.2753	1.2586
5)	6311.7	6304.0	2631.6	2624.0	9398.8	9809.5	1.2800	1.2675
6)	5926.6	5920.0	2367.8	2358.0	9558.4	9861.4	1.2477	1.2391
7)	3213.3	3229.8	2022.8	2027.8	8336.6	8414.4	1.2426	1.2410
8)	5913.5	5910.2	2684.8	2675.9	10882.4	11168.8	1.2467	1.2396

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 6.0% for case no. 4

9 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6340.0	6334.6	2658.3	2650.0	9588.2	10065.1	1.2772	1.2633
2)	6397.8	6389.3	2692.0	2683.1	9591.8	10064.5	1.2807	1.2666
3)	6439.9	6430.8	2612.9	2601.8	9438.0	9985.2	1.2768	1.2606
4)	6528.8	6516.2	2545.0	2532.0	9012.6	9655.3	1.2824	1.2622
5)	6472.9	6462.5	2725.7	2716.2	9527.3	10054.9	1.2861	1.2701
6)	6046.8	6040.1	2446.8	2436.4	9708.1	10051.0	1.2520	1.2424
7)	3360.8	3377.3	2131.6	2136.8	8748.2	8824.8	1.2437	1.2421
8)	6023.8	6020.9	2764.2	2755.0	11056.8	11372.8	1.2500	1.2422

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 7.1% for case no. 4

9.5 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6483.0	6475.7	2747.8	2737.9	9702.7	10283.9	1.2832	1.2662
2)	6552.6	6541.5	2785.6	2774.6	9705.6	10299.6	1.2870	1.2694
3)	6582.8	6571.5	2702.9	2689.9	9532.4	10192.3	1.2835	1.2639
4)	6676.3	6660.7	2635.9	2620.5	9079.9	9856.3	1.2903	1.2659
5)	6633.7	6619.7	2821.1	2809.0	9625.1	10296.9	1.2931	1.2728
6)	6167.4	6160.4	2527.3	2516.3	9850.7	10239.3	1.2566	1.2457
7)	3510.0	3526.1	2240.8	2246.1	9169.4	9243.4	1.2444	1.2430
8)	6133.7	6131.0	2844.7	2835.1	11224.7	11573.8	1.2534	1.2450

Max abs pct diff in TEMPERATURE = 0.5% for case no. 7
Max abs pct diff in BALLERGY = 8.6% for case no. 4

10 kJ/g added

	T(Std)	T(Ext)	Imp(Std)	Imp(Ext)	Ball(Std)	Ball(Ext)	Gam(Std)	Gam(Ext)
1)	6626.4	6616.5	2838.8	2826.9	9794.6	10500.9	1.2898	1.2692
2)	6707.6	6692.8	2880.6	2867.0	9790.1	10531.8	1.2942	1.2722
3)	6727.0	6712.7	2794.8	2779.4	9604.0	10398.5	1.2910	1.2673
4)	6825.8	6806.2	2729.0	2710.7	9120.9	10057.8	1.2992	1.2695
5)	6794.6	6775.8	2917.9	2902.5	9687.6	10535.7	1.3012	1.2755
6)	6288.3	6281.0	2609.4	2597.5	9985.4	10426.3	1.2613	1.2491
7)	3659.8	3675.3	2349.8	2355.0	9597.0	9667.9	1.2448	1.2436
8)	6243.4	6240.8	2926.3	2916.3	11385.9	11772.0	1.2570	1.2477

Max abs pct diff in TEMPERATURE = 0.4% for case no. 7
Max abs pct diff in BALLERGY = 10.3% for case no. 4

GRAND TOTALS

MEAN ABSOLUTE DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
7.5	6.0	176.9

MEAN ABSOLUTE PERCENT DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
0.174	0.31	2.01

ROOT MEAN SQUARE DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
8.3	6.7	262.0

ROOT MEAN SQUARE PERCENT DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
0.20	0.32	2.8

Appendix G.

Output from COMPARE.BAS: The Effects of Excluding/Including Ions with McBride's Extended Library

The two EXMUCET output files are TSTLBONO.EXT and TSTLBOIO.EXT

The input (SUMMARY) files are TSTLBSNO.EXT and TSTLBSIO.EXT

Thermo library used for first set was
*** B. McBride's EXTENDED-RANGE Library ***

Thermo library used for second set was
*** B. McBride's EXTENDED-RANGE Library ***

Number of energies = 21

0 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	3010.2	3010.2	1077.9	1077.9	4583.2	4583.2	1.2352	1.2352
2)	2549.1	2549.1	943.5	943.5	3736.5	3736.5	1.2525	1.2525
3)	3392.2	3392.2	1136.3	1136.3	5184.0	5184.0	1.2192	1.2192
4)	3811.9	3811.9	1173.5	1173.5	5723.1	5723.1	1.2050	1.2050
5)	2490.6	2490.6	927.9	927.9	3588.6	3588.6	1.2586	1.2586
6)	3738.6	3738.6	1198.2	1198.2	6278.9	6278.9	1.1908	1.1908
7)	1216.5	1216.5	472.6	472.6	2899.8	2899.8	1.1630	1.1630
8)	3574.6	3574.6	1382.5	1382.5	6590.0	6590.1	1.2098	1.2098

Max abs pct diff in TEMPERATURE = 0.00% for case no. 1
Max abs pct diff in BALLERGY = 0.00% for case no. 8

2 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	4081.4	4081.4	1482.8	1482.8	6410.5	6410.6	1.2313	1.2313
2)	3774.5	3774.5	1406.5	1406.5	5794.3	5794.4	1.2427	1.2427
3)	4329.4	4329.4	1487.0	1487.0	6738.9	6738.9	1.2207	1.2207
4)	4521.1	4521.1	1457.0	1457.0	6802.2	6802.3	1.2142	1.2142
5)	3745.4	3745.4	1404.3	1404.3	5661.6	5661.6	1.2480	1.2480
6)	4315.5	4315.5	1451.5	1451.5	7255.3	7255.3	1.2001	1.2001
7)	1562.4	1562.4	735.3	735.3	3886.6	3886.6	1.1892	1.1892
8)	4301.6	4301.6	1706.7	1706.7	8062.8	8062.8	1.2117	1.2117

Max abs pct diff in TEMPERATURE = 0.00% for case no. 1
Max abs pct diff in BALLERGY = 0.00% for case no. 2

4 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	4844.6	4844.6	1820.6	1820.6	7681.0	7680.9	1.2370	1.2370
2)	4709.6	4709.6	1796.3	1796.3	7360.3	7360.3	1.2441	1.2441
3)	5002.4	5002.4	1793.8	1793.8	7810.4	7810.4	1.2297	1.2297
4)	5106.4	5106.4	1737.1	1737.1	7653.2	7653.1	1.2270	1.2270
5)	4715.9	4715.9	1807.2	1807.2	7266.4	7266.4	1.2487	1.2487
6)	4828.6	4828.6	1710.9	1710.9	8099.2	8099.2	1.2112	1.2112
7)	1974.5	1974.5	1081.3	1081.3	4984.6	4984.6	1.2169	1.2169
8)	4857.9	4857.8	2000.6	2000.6	9159.6	9159.6	1.2184	1.2184

Max abs pct diff in TEMPERATURE = 0.00% for case no. 8
Max abs pct diff in BALLERGY = 0.00% for case no. 4

6 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	5471.3	5471.2	2144.3	2144.2	8698.6	8698.5	1.2465	1.2465
2)	5439.3	5439.2	2150.2	2150.2	8557.6	8557.5	1.2513	1.2513
3)	5588.0	5587.9	2103.1	2103.0	8716.4	8716.3	1.2413	1.2413
4)	5667.2	5667.1	2036.1	2036.0	8456.3	8456.2	1.2408	1.2408
5)	5476.2	5476.2	2171.7	2171.7	8502.0	8501.9	1.2554	1.2554
6)	5318.5	5318.5	1986.2	1986.2	8896.4	8896.3	1.2233	1.2233
7)	2515.2	2515.2	1495.9	1495.9	6456.5	6456.5	1.2317	1.2317
8)	5343.9	5343.8	2294.1	2294.1	10099.8	10099.6	1.2271	1.2271

Max abs pct diff in TEMPERATURE = 0.00% for case no. 8
Max abs pct diff in BALLERGY = 0.00% for case no. 8

8 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	6051.3	6051.1	2477.5	2477.4	9621.7	9621.4	1.2575	1.2575
2)	6081.8	6081.6	2502.8	2502.7	9584.0	9583.7	1.2611	1.2611
3)	6150.6	6150.3	2430.1	2430.0	9568.6	9568.2	1.2540	1.2540
4)	6230.5	6230.2	2360.1	2359.9	9254.8	9254.4	1.2550	1.2550
5)	6144.0	6143.8	2532.6	2532.5	9560.2	9559.9	1.2649	1.2649
6)	5800.1	5799.9	2281.1	2281.0	9671.0	9670.6	1.2359	1.2359
7)	3084.2	3084.2	1919.6	1919.6	8013.3	8013.3	1.2396	1.2396
8)	5799.1	5799.0	2597.9	2597.8	10962.1	10961.8	1.2370	1.2370

Max abs pct diff in TEMPERATURE = 0.00% for case no. 3
Max abs pct diff in BALLERGY = 0.00% for case no. 4

10 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	6617.0	6616.5	2827.2	2826.9	10501.7	10500.9	1.2692	1.2692
2)	6693.2	6692.8	2867.3	2867.0	10532.5	10531.8	1.2722	1.2722
3)	6713.3	6712.7	2779.7	2779.4	10399.3	10398.5	1.2673	1.2673
4)	6807.0	6806.2	2711.1	2710.7	10058.8	10057.8	1.2695	1.2695
5)	6776.3	6775.8	2902.8	2902.5	10536.4	10535.7	1.2755	1.2755
6)	6281.4	6281.0	2597.7	2597.5	10427.0	10426.3	1.2491	1.2491
7)	3675.3	3675.3	2355.0	2355.0	9667.9	9667.9	1.2436	1.2436
8)	6241.1	6240.8	2916.5	2916.3	11772.6	11772.0	1.2477	1.2477

Max abs pct diff in TEMPERATURE = 0.01% for case no. 4
Max abs pct diff in BALLERGY = 0.01% for case no. 4

12 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	7179.5	7178.4	3193.1	3192.5	11354.1	11352.6	1.2812	1.2812
2)	7292.8	7291.9	3244.5	3244.0	11437.1	11435.8	1.2837	1.2837
3)	7284.7	7283.6	3151.8	3151.1	11216.7	11215.1	1.2810	1.2810
4)	7400.1	7398.6	3087.9	3087.0	10869.3	10867.3	1.2841	1.2841
5)	7390.3	7389.3	3281.4	3280.8	11466.6	11465.0	1.2862	1.2862
6)	6768.4	6767.6	2937.6	2937.1	11159.7	11158.6	1.2632	1.2632
7)	4257.2	4257.2	2780.0	2780.0	11363.7	11363.7	1.2446	1.2446
8)	6679.3	6678.7	3252.2	3251.7	12536.1	12535.1	1.2594	1.2594

Max abs pct diff in TEMPERATURE = 0.02% for case no. 4
Max abs pct diff in BALLERGY = 0.02% for case no. 4

14 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	7738.3	7736.3	3570.7	3569.5	12181.8	12179.1	1.2931	1.2931
2)	7879.6	7877.6	3627.9	3626.7	12308.3	12305.7	1.2948	1.2947
3)	7863.8	7861.6	3542.1	3540.7	12020.0	12017.2	1.2947	1.2946
4)	8006.1	8003.2	3485.2	3483.5	11685.0	11681.4	1.2983	1.2982
5)	7981.9	7979.8	3660.0	3658.7	12362.5	12359.6	1.2961	1.2960
6)	7265.4	7264.1	3301.2	3300.2	11859.2	11857.3	1.2784	1.2783
7)	4792.3	4792.3	3182.0	3182.0	12958.8	12958.8	1.2455	1.2455
8)	7119.1	7118.1	3605.8	3605.1	13246.9	13245.4	1.2722	1.2722

Max abs pct diff in TEMPERATURE = 0.04% for case no. 4
Max abs pct diff in BALLERGY = 0.03% for case no. 4

16 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	8285.8	8282.5	3952.6	3950.5	12984.1	12979.8	1.3044	1.3044
2)	8442.5	8439.0	4007.5	4005.3	13149.9	13145.4	1.3048	1.3047
3)	8441.0	8437.0	3942.0	3939.5	12806.4	12801.9	1.3078	1.3077
4)	8612.2	8607.2	3893.6	3890.5	12504.2	12498.3	1.3114	1.3113
5)	8540.0	8536.2	4029.3	4027.0	13231.6	13226.5	1.3045	1.3045
6)	7774.9	7772.5	3688.1	3686.4	12511.0	12508.4	1.2948	1.2947
7)	5278.5	5278.5	3566.1	3566.1	14408.9	14408.9	1.2475	1.2475
8)	7563.7	7562.0	3977.4	3976.1	13892.6	13890.5	1.2863	1.2862

Max abs pct diff in TEMPERATURE = 0.06% for case no. 4
Max abs pct diff in BALLERGY = 0.05% for case no. 4

18 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	8812.9	8807.5	4331.5	4328.1	13762.2	13755.8	1.3147	1.3146
2)	8972.0	8966.2	4376.6	4373.1	13970.1	13963.0	1.3133	1.3132
3)	9001.8	8995.3	4341.5	4337.3	13576.0	13569.1	1.3198	1.3196
4)	9201.1	9192.9	4301.5	4296.3	13327.2	13318.1	1.3228	1.3226
5)	9059.1	9053.0	4385.7	4382.0	14087.0	14078.6	1.3113	1.3113
6)	8296.3	8292.3	4096.4	4093.5	13098.1	13094.8	1.3127	1.3126
7)	5726.1	5726.1	3940.2	3940.2	15716.9	15716.8	1.2507	1.2507
8)	8014.0	8011.3	4366.0	4363.8	14456.2	14453.7	1.3020	1.3019

Max abs pct diff in TEMPERATURE = 0.09% for case no. 4
Max abs pct diff in BALLERGY = 0.07% for case no. 4

20 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	9313.7	9305.6	4703.6	4698.3	14522.3	14513.4	1.3239	1.3237
2)	9465.9	9457.2	4734.3	4728.8	14785.6	14774.6	1.3202	1.3201
3)	9534.9	9525.0	4733.2	4726.7	14337.1	14327.3	1.3301	1.3299
4)	9759.1	9746.7	4700.6	4692.7	14162.7	14149.0	1.3319	1.3317
5)	9541.3	9532.2	4730.8	4725.2	14948.9	14935.8	1.3165	1.3164
6)	8826.3	8819.9	4522.3	4517.5	13602.5	13599.4	1.3325	1.3322
7)	6145.3	6145.2	4310.3	4310.2	16892.1	16892.0	1.2552	1.2552
8)	8469.3	8465.1	4769.7	4766.3	14918.5	14916.3	1.3197	1.3195

Max abs pct diff in TEMPERATURE = 0.1% for case no. 4
Max abs pct diff in BALLERGY = 0.10% for case no. 4

22 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	9787.7	9776.1	5068.6	5060.8	15277.8	15265.9	1.3318	1.3315
2)	9928.0	9915.5	5083.3	5075.2	15620.2	15603.9	1.3254	1.3253
3)	10036.4	10021.9	5115.2	5105.5	15110.5	15096.7	1.3385	1.3382
4)	10281.5	10263.8	5088.6	5077.0	15034.1	15013.8	1.3385	1.3382
5)	9992.5	9979.6	5068.5	5060.3	15843.4	15823.5	1.3199	1.3198
6)	9358.8	9348.9	4960.9	4953.4	14010.5	14009.4	1.3541	1.3536
7)	6543.9	6543.7	4680.1	4680.0	17939.4	17939.0	1.2609	1.2609
8)	8927.6	8921.3	5186.2	5180.9	15260.5	15260.3	1.3398	1.3395

Max abs pct diff in TEMPERATURE = 0.2% for case no. 4
Max abs pct diff in BALLERGY = 0.1% for case no. 4

24 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	10238.1	10222.1	5428.9	5417.8	16050.8	16035.6	1.3382	1.3379
2)	10364.2	10347.0	5427.2	5415.7	16505.6	16482.0	1.3288	1.3286
3)	10508.4	10488.3	5489.2	5475.4	15931.2	15912.0	1.3446	1.3441
4)	10770.9	10746.7	5466.9	5450.6	15984.8	15954.9	1.3420	1.3416
5)	10419.1	10401.6	5402.4	5391.0	16803.2	16773.9	1.3215	1.3214
6)	9887.2	9872.3	5407.2	5395.7	14319.8	14324.6	1.3776	1.3767
7)	6927.3	6927.0	5052.1	5051.8	18857.4	18856.7	1.2679	1.2679
8)	9386.2	9376.9	5613.2	5605.2	15467.2	15472.1	1.3629	1.3623

Max abs pct diff in TEMPERATURE = 0.2% for case no. 4
Max abs pct diff in BALLERGY = 0.2% for case no. 4

26 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	10669.7	10648.3	5787.1	5771.9	16876.9	16858.0	1.3429	1.3424
2)	10779.7	10756.9	5769.0	5753.4	17484.4	17451.0	1.3300	1.3297
3)	10955.6	10928.8	5857.7	5838.8	16852.6	16825.9	1.3476	1.3470
4)	11232.5	11200.5	5838.0	5815.9	17083.8	17039.5	1.3417	1.3413
5)	10826.4	10803.3	5735.4	5719.8	17871.7	17829.5	1.3209	1.3208
6)	10406.0	10384.3	5857.6	5840.4	14550.2	14567.2	1.4026	1.4009
7)	7299.3	7298.7	5427.4	5426.8	19639.7	19638.7	1.2763	1.2763
8)	9843.1	9829.6	6049.0	6037.3	15532.3	15547.9	1.3894	1.3883

Max abs pct diff in TEMPERATURE = 0.3% for case no. 4
Max abs pct diff in BALLERGY = 0.3% for case no. 4

28 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	11086.8	11058.6	6145.5	6124.9	17814.7	17790.6	1.3450	1.3443
2)	11178.7	11149.1	6110.8	6089.9	18616.0	18569.7	1.3283	1.3279
3)	11382.5	11347.5	6222.8	6197.4	17954.3	17917.2	1.3466	1.3459
4)	11670.7	11629.5	6202.7	6173.7	18435.7	18369.9	1.3365	1.3361
5)	11218.1	11188.3	6068.8	6048.1	19109.2	19049.7	1.3176	1.3175
6)	10912.2	10881.7	6309.6	6284.8	14757.7	14796.0	1.4275	1.4248
7)	7662.4	7661.4	5807.0	5806.0	20276.6	20275.3	1.2864	1.2864
8)	10296.9	10277.8	6493.1	6476.1	15465.9	15501.6	1.4198	1.4178

Max abs pct diff in TEMPERATURE = 0.4% for case no. 4
Max abs pct diff in BALLERGY = 0.4% for case no. 4

30 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	11492.5	11455.9	6504.6	6477.3	18964.9	18930.9	1.3430	1.3422
2)	11563.6	11526.0	6452.8	6425.3	19985.2	19921.7	1.3229	1.3225
3)	11791.3	11746.7	6584.0	6550.9	19355.2	19302.4	1.3402	1.3394
4)	12087.0	12035.2	6559.1	6522.0	20195.5	20096.2	1.3248	1.3245
5)	11596.3	11558.6	6402.7	6375.7	20600.2	20517.8	1.3108	1.3107
6)	11404.3	11362.4	6761.2	6726.3	15059.8	15129.8	1.4490	1.4446
7)	8018.5	8016.8	6191.4	6189.8	20756.0	20754.7	1.2983	1.2982
8)	10747.5	10720.8	6945.3	6920.9	15309.8	15378.8	1.4537	1.4500

Max abs pct diff in TEMPERATURE = 0.4% for case no. 4
Max abs pct diff in BALLERGY = 0.5% for case no. 4

32 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	11886.9	11840.3	6861.7	6826.4	20505.2	20444.7	1.3346	1.3339
2)	11934.9	11887.8	6793.2	6757.9	21712.3	21625.5	1.3129	1.3125
3)	12181.6	12125.9	6937.9	6895.6	21233.4	21152.4	1.3267	1.3260
4)	12478.8	12415.3	6900.7	6854.9	22588.7	22430.4	1.3055	1.3056
5)	11961.3	11914.4	6735.3	6700.8	22463.1	22349.6	1.2998	1.2998
6)	11879.0	11822.7	7206.7	7159.1	15687.3	15791.8	1.4594	1.4533
7)	8368.9	8366.3	6581.3	6578.7	21064.5	21064.0	1.3124	1.3123
8)	11194.6	11157.7	7404.7	7370.3	15171.7	15289.5	1.4881	1.4820

Max abs pct diff in TEMPERATURE = 0.5% for case no. 4
Max abs pct diff in BALLERGY = 0.8% for case no. 8

34 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	12265.7	12208.2	7208.6	7165.0	22752.7	22614.3	1.3168	1.3168
2)	12290.8	12232.8	7127.8	7083.4	23969.7	23844.9	1.2974	1.2971
3)	12548.7	12481.0	7276.0	7224.2	23854.2	23708.9	1.3050	1.3047
4)	12838.6	12764.0	7215.5	7162.4	25936.2	25655.9	1.2782	1.2792
5)	12311.2	12253.9	7062.1	7019.0	24863.9	24703.1	1.2840	1.2841
6)	12326.3	12254.2	7631.5	7570.3	17084.0	17180.3	1.4467	1.4406
7)	8714.8	8710.8	6977.3	6973.4	21187.9	21190.0	1.3293	1.3291
8)	11635.2	11585.4	7866.0	7818.7	15307.3	15475.2	1.5139	1.5052

Max abs pct diff in TEMPERATURE = 0.6% for case no. 6
Max abs pct diff in BALLERGY = 1.1% for case no. 8

36 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	12617.3	12550.1	7528.6	7479.1	26237.6	25886.2	1.2869	1.2889
2)	12626.3	12556.9	7448.3	7394.4	27002.8	26799.9	1.2758	1.2759
3)	12883.3	12804.8	7584.3	7525.1	27599.0	27291.7	1.2748	1.2757
4)	13154.4	13072.1	7486.7	7431.0	30658.7	30111.5	1.2442	1.2468
5)	12641.4	12573.0	7375.4	7323.4	28034.7	27786.7	1.2631	1.2636
6)	12724.9	12640.3	8006.7	7936.9	20011.7	19921.3	1.4001	1.3984
7)	9057.2	9051.4	7380.7	7374.8	21111.5	21119.6	1.3496	1.3492
8)	12058.3	11994.1	8312.3	8251.5	16285.1	16430.7	1.5104	1.5022

Max abs pct diff in TEMPERATURE = 0.7% for case no. 6
Max abs pct diff in BALLERGY = 1.8% for case no. 4

38 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	12923.0	12851.6	7797.2	7749.0	31637.3	30825.5	1.2465	1.2514
2)	12933.1	12853.4	7742.1	7680.7	31149.4	30766.7	1.2485	1.2496
3)	13172.7	13088.1	7844.5	7784.3	32926.6	32258.1	1.2382	1.2413
4)	13415.3	13332.0	7699.0	7648.9	37147.8	36105.1	1.2073	1.2119
5)	12944.0	12865.6	7663.4	7604.2	32290.6	31858.8	1.2373	1.2387
6)	13049.0	12961.5	8298.0	8232.1	25333.3	24710.3	1.3276	1.3331
7)	9397.3	9389.0	7792.8	7784.2	20821.0	20840.6	1.3743	1.3735
8)	12438.5	12363.9	8707.8	8639.7	19125.9	18994.2	1.4553	1.4549

Max abs pct diff in TEMPERATURE = 0.7% for case no. 6
Max abs pct diff in BALLERGY = 2.8% for case no. 4

40 kJ/g added

	T(no)	T(ions)	Imp(no)	Imp(ion)	Ball(no)	Ball(ion)	Gam(no)	Gam(ion)
1)	13169.0	13100.7	7996.9	7958.8	39349.4	37832.6	1.2032	1.2104
2)	13200.9	13114.9	7993.5	7930.4	36797.3	36040.3	1.2172	1.2200
3)	13408.3	13324.6	8044.0	7991.5	40147.0	38868.1	1.2004	1.2056
4)	13619.9	13542.0	7849.6	7812.3	45484.4	43748.9	1.1726	1.1786
5)	13209.4	13124.8	7911.2	7850.3	37994.7	37196.7	1.2082	1.2110
6)	13291.2	13210.8	8495.5	8444.9	33274.1	31838.4	1.2553	1.2652
7)	9736.1	9724.6	8215.2	8202.8	20302.5	20342.8	1.4046	1.4032
8)	12746.4	12671.2	9011.9	8949.9	24833.7	24038.9	1.3629	1.3723

Max abs pct diff in TEMPERATURE = 0.7% for case no. 2
Max abs pct diff in BALLERGY = 4.3% for case no. 6

GRAND TOTALS

MEAN ABSOLUTE DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
20.7	15.3	105.2

MEAN ABSOLUTE PERCENT DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
0.174	0.22	0.36

ROOT MEAN SQUARE DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
34.6	25.7	297.4

ROOT MEAN SQUARE PERCENT DEVIATIONS

Temp (K)	Impetus (J/g)	Ballergy (J/g)
0.28	0.35	0.9

Appendix H.

Comparison of the Species

with Mole Fractions Greater than 1.0×10^{-7}

Produced by Two Different Thermo Libraries

NOTE: These products are for Composition No. 1 with 5000 J/g of added Energy.

OLD (STD) LIB		NEW (EXTENDED) LIB		OLD (STD) LIB		NEW (EXTENDED) LIB	
C2H2	3.936E-07	C2H2	3.391E-07	CH3OH	1.569E-07	CH3OH	1.509E-07
C	2.005E-06	C	2.031E-06	N	3.874E-04	N	3.873E-04
C2H RAD	2.412E-07	C2H	1.251E-07	N2	2.488E-01	N2	2.494E-01
CCO RAD	2.128E-06	CCO RAD	1.685E-06	N2H2	1.847E-06	N2H2	1.789E-06
CH	2.979E-06	CH	2.642E-06	N2O	4.212E-05	N2O	4.106E-05
CH2	4.722E-06	CH2	4.812E-06	N3	2.328E-07	N3	2.303E-07
CH3	5.728E-06	CH3	5.250E-06	N3H	2.425E-07	N3H	2.372E-07
CH4	1.553E-06	CH4	1.830E-06	NCN RAD	2.704E-07	NCN	1.931E-05
CN	4.147E-05	CN	3.729E-05	NCO	2.678E-05	NCO	1.752E-05
CO	2.813E-01	CO	2.823E-01	NH	8.050E-04	NH	5.215E-04
CO2	3.857E-02	CO2	3.774E-02	NH2	4.908E-04	NH2	4.789E-04
CH2O	8.209E-05	CH2O	6.732E-05	NH2OH	3.052E-06	NH2OH	2.880E-06
HCOOH	8.562E-05	HCOOH	8.320E-05	NH3	3.109E-04	NH3	4.012E-04
H	4.489E-02	H	4.477E-02	NO	1.746E-02	NO	1.712E-02
H2	1.335E-01	H2	1.316E-01	NO2	4.068E-05	NO2	3.892E-05
H2N2	1.113E-06	- - -	- - - -	O	8.990E-03	O	8.842E-03
H2O	1.680E-01	H2O	1.708E-01	O2	4.309E-03	O2	4.179E-03
H2O2	7.128E-05	H2O2	8.200E-05	O3	1.912E-07	O3	6.246E-07
HCN	3.197E-04	HCN	3.241E-04	OH	4.982E-02	OH	4.877E-02
HCO RAD	1.053E-03	HCO	1.035E-03	- - -	- - - -	CH2OH	1.584E-06
HNCO	8.314E-05	HNCO	8.182E-05	- - -	- - - -	CNN	1.957E-06
HNO	2.890E-04	HNO	2.999E-04	- - -	- - - -	CHCO	2.409E-07
HNO2	2.549E-05	HNO2	2.410E-05	- - -	- - - -	COOH	2.663E-04
HO2	2.487E-04	HO2	2.332E-04	- - -	- - - -	HNC	1.368E-05
CH3O	9.268E-07	- - -	- - - -	- - -	- - - -	CH3O	1.734E-07
KETENE	3.037E-07	KETENE	2.735E-07				

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Appendix I.

Listing of Thermodynamic Tables Supplied by NIST

ARL Requested COEFS for	NIST Sent Tables for	ARL Requested COEFS for	NIST Sent Tables for
C	Carbon, monatomic	N2	- - - - - - - -
C+	Carbon, unipositive	N+	Nitrogen, unipositive
C-	Carbon, uninegative	N2+	- - - - - - - -
C2	CCH (g) Radical	N2-	- - - - - - - -
C2-	- - - - - - -	N2O+	- - - - - - - -
CH	CH (g)	NO	NO (g)
CH+	CH+ (g)		NO+ (g)
CH2	CH2 (g)		NO2 (g)
CN	CN (g)		NO2- (g)
CN+	CN+ (g)	O	Oxygen, monatomic
CN-	CN- (g)	O+	Oxygen, unipositive
CO	- - - - - - -	O-	Oxygen, uninegative
CO2-	CO2- (g)	O2	- - - - - - -
---	electron gas	O2-	- - - - - - -
---	Hydrogen, monatomic	OH	OH (g)
H+	Hydrogen, unipositive	OH+	OH+ Hydroxyl positive
H-	Hydrogen, uninegative	OH-	OH- Hydroxide
H2+	- - - - - - -	ONO-	- - - - - - - - - -
H2-	- - - - - - -	Ti	Titanium, monatomic
N	Nitrogen, monatomic	Ti+	Titanium, unipositive
N-	Nitrogen, uninegative	TiO	TiO (g)
		----	Titanium, uninegative

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Appendix J.

Comparison of Thermodynamic Tables

Produced by Back-Calculation from the LRC Coefficients

with Those Furnished by NIST

Units are Joules, moles, and Kelvins

NAME/	HEAT CAPACITY		ENTROPY		ENTHALPY		Number
	MnAvDev	Pct RMS	MnAvDev	Pct RMS	MnAvDev	Pct RMS	of Pts
C+	Carbon, unipositive ion						
	0.002	0.020	0.000	0.001	1.2	0.00	102
electron gas							
	0.004	0.019	-0.000	0.005	0.0	0.01	102
H+	Hydrogen, unipositive ion						
	0.004	0.019	-0.000	0.002	0.0	0.01	102
H-	Hydrogen, uninegative ion						
	0.004	0.019	-0.000	0.002	0.0	0.01	102
O	Oxygen, monatomic						
	-0.001	0.073	-0.002	0.002	-8.3	0.01	102
O+	Oxygen, unipositive ion						
	0.001	0.029	0.001	0.002	1.1	0.01	102
N+	Nitrogen, unipositive ion						
	0.000	0.016	0.001	0.001	0.3	0.01	102
N-	Nitrogen, uninegative ion						
	0.001	0.015	0.001	0.001	0.2	0.01	102
N	Nitrogen, monatomic						
	-0.003	0.097	-0.000	0.002	-18.1	0.02	102
H	Hydrogen, monatomic						
	-0.001	0.167	-0.003	0.003	-17.0	0.03	102
O-	Oxygen, uninegative ion						
	-0.001	0.026	0.002	0.002	-11.1	0.03	102

C Carbon, monatomic

0.007	0.268	-0.004	0.004	-26.3	0.04	102

OH- Hydroxyl negative ion

0.133	0.409	0.052	0.032	407.3	0.20	102

NO2- Nitrogen dioxide negative ion

0.331	1.090	-0.656	0.207	221.0	0.52	62

CN- Cyanide

0.133	0.461	1.131	0.405	795.9	0.58	102

CH2 Methylene

-0.070	0.907	1.103	0.393	419.9	0.72	62

NO+ Nitric oxide positive ion

0.969	5.001	0.186	0.103	1221.3	0.75	102

OH Hydroxyl

-1.654	9.444	0.187	0.148	3.7	1.07	102

NO Nitric oxide

1.668	7.135	0.409	0.213	2798.2	1.58	102

OH+ Hydroxyl positive ion

0.858	4.395	0.925	0.423	4616.5	2.24	102

CN Cyanogen

1.794	5.198	1.042	0.430	5074.3	2.29	102

CH Methylidyne

-3.148	12.080	-0.999	0.480	-5007.8	2.69	102

CCH Ethynyl Radical

-1.749	5.545	9.548	2.966	-3400.1	4.20	102

NO2 Nitrogen dioxide

4.763	10.896	3.027	1.007	7630.9	4.43	62

C- Carbon, uninegative ion

-3.654	17.626	-1.720	1.188	-5994.0	8.22	62

CN+ Cyanogen, ion

1.978	8.993	-5.291	2.514	13159.2	10.87	102

CH+ Methylidyne, ion

3.852	23.368	8.505	3.711	30723.0	16.33	102

Appendix K.

Listing of Program TIGFIT5

```
      PROGRAM TIGFIT5

C
C  This version: 26 January 1993

C  Specifically adapted to creating coefficients for EXBLAKE.  This
C  program is the fifth of a series of programs named either TIGFITi
C  or TIGFITiX (i = 1,6).  This program is specifically designed to
C  get its input data from the tables given to ARL/WTD/APCB by Ms.
C  Bonnie McBride (NASA Lewis Research Center).  Her tables have 9
C  columns per temperature.  For use with this program they have been
C  copied into TABLES.IN; the sentinel line,
C        9999., 999., 99., 9., 0.9, 0.09  , 99., 99., 99.
C  has been added, and the title line (which contains the name of the
C  species) has been changed.  A '$' has been placed in col 1 as a
C  sentinel, and the name of the species starts in col 8.

C  See TIGFIT6 for a version designed for input from the JANAF Tables
C  tape.  It would not be difficult to modify the present program to
C  accept one or the other of these inputs, but it is easier to have a
C  separate program.

C  This one has all of the features of TIGFIT4 (use of the '$'
C  sentinel; computation of measures of goodness-of-fit);  A N D  it
C  includes the cut-off at 15 000 K.

C  See the Comments at the beginning of TIGFIT4 for further details.

C  In this version, the output files have been changed from TIGFIT.OUT
C  and TIGFIT.AUX to TIGFIT5.OUT and TIGFIT5.AUX.

      IMPLICIT REAL*8 (A-H,O-Z)
C
      DIMENSION A(7,7), B(9), KX(7), JUNK(80)
      DIMENSION TK(500), CPP(500), SS(500), HH(500)

      CHARACTER XNAME*10,PHASE*6, JUNK*1, SENT*1
      PARAMETER (N6=0)
      LOGICAL HITEMP

      COMMON /COEFS/ B, NUM
      COMMON /FUNCS/ TK, CPP, SS, HH, TFIX, TSTART, ENTRP0, HOFJ,
     $ XNAME, PHASE
      COMMON /IOSTUF/ LI, LO
      COMMON /LSTSQ/ T, T2, T3, T4, T5, T6, TM2, TM3, TM4, TM5, TM6,
```

```
     $  Y, YT2, YT3, TM, SN, YTM2, YT, YTM, YTM3

        DATA PHASE/ 'GAS   ' /
C
       LO = 6
       LI = 5
        OPEN (LI,FILE='TEMPS.IN',STATUS='OLD')
        OPEN (3,FILE='TIGFIT5.OUT',STATUS='UNKNOWN')
        OPEN (LO,FILE='TIGFIT5.AUX',STATUS='UNKNOWN')
        OPEN (4,FILE='CHEKK5',STATUS='UNKNOWN')
        OPEN (2,FILE='CALORIC',ACCESS='APPEND')
        WRITE (2, 81)
   81 FORMAT (' The data cards for the TIGER code are (units = calories'
     $ ', mols, & K): ')
C
C       CALL LOGO
C
       REWIND LI
       READ (LI, *, END=33) TFIX, TSTART
       CLOSE (LI)
       OPEN (LI,FILE='TABLES.IN',STATUS='OLD')
       REWIND LI
   10 READ(LI,1020,END=33) SENT, XNAME
 1020 FORMAT(A1,6X, A6 )
       IF (SENT .NE. '$') GOTO 10

        WRITE (N6,2008) XNAME
 2008   FORMAT(1X,'Processing ==> ',A10)
C  Initialize the elements that will make up the matrix
       CALL FMATR (0, X1, X2)
C
C  Skip the header line in the table
       READ (LI, 499, END=33) JUNK
  499 FORMAT (80A1)
C  Read the first line of data.
   15 READ(LI,*, END=33) TEM, CP, X1, HMH298, ENTRP0, X2, X3, HOFJ, X4
C  Is temperature the fixed temperature? If not, read another line.
       IF (TEM. LT. TFIX-0.05 .OR. TEM .GT. TFIX+0.05 ) GOTO 15
C  Yes, it is the fixed T.  Is T Fix = T Start?
C  If it is, then start saving data and continue to read the table
   20 IF (TEM .GE. TSTART-0.05 .AND. TEM .LE. TSTART+0.05 ) THEN
                  KT=1
                  TK(1) = TSTART
                  CPP(1) = CP
                  SS(1) = ENTRP0
                  HH(1) = HMH298
                  HITEMP = .FALSE.
                  GOTO 35
       END IF
```

```
C  No, T Fix wasn't T Start.  Keep looking for T Start
   25 READ (LI,*, END=33, ERR=999) TEM, CP, X1, HMH298, ENTROP, X2,
     $  X3, ENTHALP, X4
      IF (TEM .LT. TSTART-0.05 .OR . TEM .GT. TSTART+0.05 ) GOTO 25
C  At last T Start has been found; save values and keep reading table.
   29 KT=1
      TK(1) = TSTART
      CPP(1) = CP
      SS(1) = ENTROP
      HH(1) = HMH298
      HITEMP = .FALSE.

      CALL FMATR (1, TK(1), CP)

   35 KT = KT + 1
      READ(LI,*, END=33) TEM, CP, X1, HMH298, ENTROP, X2,
     $ X3, ENTHALP, X4
      TK(KT) = TEM
      CPP(KT) = CP
      SS(KT) = ENTROP
      HH(KT) = HMH298
C          WRITE (LO,*) KT, TEM, CP, ENTROP
      IF (TEM .LE. 14999.D0) GOTO 49
      IF (TEM .GE. 15000.D0) THEN
         HITEMP = .TRUE.
         GOTO 60
      END IF

   49 IF (CP .EQ. 999.0D0)  GOTO 60
      CALL FMATR (1, TK(KT), CP)
      IF (.NOT. HITEMP) GOTO 35
   60 NUM=KT-1

      IF (HITEMP) NUM=KT

      B(1) = Y
      B(2) = YT
      B(3) = YT2
      B(4) = YT3
      B(5) = YTM
      B(6) = YTM2
      B(7) = YTM3
      A(1,1) = SN
      A(2,5) = SN
      A(3,6) = SN
      A(4,7) = SN
      A(5,2) = SN
      A(6,3) = SN
      A(7,4) = SN
```

```
      A(2,1) = T
      A(3,5) = T
      A(4,6) = T
      A(1,2) = T
      A(5,3) = T
      A(6,4) = T
      A(3,1) = T2
      A(2,2) = T2
      A(4,5) = T2
      A(1,3) = T2
      A(5,4) = T2
      A(4,1) = T3
      A(2,3) = T3
      A(1,4) = T3
      A(3,2) = T3
      A(5,1) = TM
      A(2,6) = TM
      A(3,7) = TM
      A(1,5) = TM
      A(6,2) = TM
      A(7,3) = TM
      A(6,1) = TM2
      A(2,7) = TM2
      A(5,5) = TM2
      A(1,6) = TM2
      A(7,2) = TM2
      A(7,1) = TM3
      A(5,6) = TM3
      A(1,7) = TM3
      A(6,5) = TM3
      A(2,4) = T4
      A(3,3) = T4
      A(4,2) = T4
      A(3,4) = T5
      A(4,3) = T5
      A(4,4) = T6
      A(5,7) = TM4
      A(6,6) = TM4
      A(7,5) = TM4
      A(6,7) = TM5
      A(7,6) = TM5
      A(7,7) = TM6
      CALL SOLVEX(7, A, B, KX, 0, KERR)
      IF (KERR .LE. 0)  GOTO 66
   64 STOP
   66 X= TFIX/1000.
      B(8)  =  HOFJ - TFIX * 8.31451 * ( ( ( B(4) * X / 4.0  + B(3)/
     A 3.0 ) * X  +  B(2) / 2.0 ) * X  + B(1) - ( ( B(7) / (X * 2.0)
     A + B(6)) / X  - B(5) * DLOG(X) ) / X )
```

```
      B(9)  = ENTRP0 - 8.31451 * ( ( ( B(4) * X / 3.0 + B(3) / 2.0 )
     A * X + B(2) ) * X  + B(1) * DLOG(X) - ( ( B(7) / (3.0 * X) +
     A B(6) / 2.0 ) / X  + B(5) ) / X )

      WRITE (LO, 70) XNAME, PHASE
   70 FORMAT(/5X, A10, /, 5X, 13HThe phase is , A6, / )

      WRITE (LO,22) TFIX, TSTART, ENTRP0, HOFJ
   22 FORMAT (' Fit fixed at T    =', F11.2/
     $        ' Fit starts at T   =', F11.2/
     $        ' Entropy at T Fix  =', F11.2/
     $        ' Enthalpy at T Fix =', F10.1 / )

C ***********************************************

C     WRITE (4, 71)  XNAME, PHASE
C  71 FORMAT(/5X, A10, 'Phase = ', A6/)

C     DO 9877 IJK=1,NUM,4
C     IJK1 = IJK
C     IJK2 = IJK1+3
C     IF (IJK2 .GT. NUM) IJK2 = NUM
C9877 WRITE (4, 9878) (IJ, TK(IJ), IJ=IJK1,IJK2)
C9878 FORMAT (4(I5,')',F8.1,3X))

C ***********************************************************

      WRITE (LO, 80)
   80 FORMAT (' The data cards for the TIGER code are (units = Joules, '
     $ ' mols, & K): '/)
      I=1
      WRITE (LO,90)  XNAME, PHASE, I, B(1), B(2), B(3)
      WRITE (3, 95)  XNAME, PHASE, I, B(1), B(2), B(3)
      WRITE (2, 95)  XNAME, PHASE, I, B(1), B(2), B(3)
      I = 2
      WRITE (LO,90)  XNAME, PHASE, I, B(4), B(5), B(6)
      WRITE (3, 95)  XNAME, PHASE, I, B(4), B(5), B(6)
      WRITE (2, 95)  XNAME, PHASE, I, B(4), B(5), B(6)
      I = 3
      WRITE (LO,90)  XNAME, PHASE, I, B(7), B(8), B(9)
      WRITE (3, 95)  XNAME, PHASE, I, B(7), B(8), B(9)
      B8 = B(8)/4.184D0
      B9 = B(9)/4.184D0
      WRITE (2, 95)  XNAME, PHASE, I, B(7), B8, B9
   90 FORMAT(5X, 5HSTR, , A6 , ',', A6, ',' ,I2, 3(2H, ,1PD14.7))
   95 FORMAT(    5HSTR, , A6 , ',', A6, ',', I2, 3(2H, ,1PD14.7))

C     WRITE (4, 110)
  110 FORMAT(/'      T           CP           S          '
```

```
     $ 'H-H298       MU/RT')
  120 FORMAT(1X,F8.2,F15.3,F15.3,F14.3,F14.4)

      T = 298.15
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120)  T, CP, S, H
      T = 300.0
      DO  130  I = 1, 18
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120) T, CP, S, H, UU
  130 T = T + 100.0
C     WRITE (LO, 70)  XNAME, PHASE
C     WRITE (LO, 110)
      DO 140  I = 1, 30
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120) T, CP, S, H, UU
  140 T = T + 100.0
C     GOTO 10
      T = 6000.0
      DO 150  I = 1,9
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120) T, CP, S, H, UU
  150 T = T + 1000.0

      CALL GOODF5

      GO TO 10

  999 WRITE (LO, *) TEM, CP, X1, HMH298, ENTROP, X2
      WRITE (4, *) TEM, CP, X1, HMH298, ENTROP, X2
   33 STOP

      END
      SUBROUTINE SOLVEX(N, A, B, KX, K, KERR)
C
C
       IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(7,7), B(9), KX(7), T(7)
      EPS = 0.0
      KERR = 0
      IF (K)   10, 10, 160
   10 DO 20   J = 1, N
   20 KX(J) = J
      DO 150   I = 1, N
      IM1 = I - 1
      IF (IM1)   50, 50, 30
   30 DO 40   J = 1, IM1
      KJ = KX(J)
      Q = A(I, KJ)
```

```
      JP1 = J + 1
      DO 40   L = JP1, N
      KL = KX(L)
   40 A(I, KL) = A(I, KL) - Q * A(J, KL)
   50 KI = KX(I)
      Q = DABS(A(I, KI))
      IF (N - I)   100, 100, 60
   60 L = I
      IP1 = I + 1
      DO 80   J = IP1, N
      KJ = KX(J)
      AIKJ = DABS(A(I, KJ))
      IF (AIKJ - Q)   80, 80, 70
   70 Q = AIKJ
      L = J
   80 CONTINUE
      IF (L - I)   90, 100, 90
   90 J = KX(L)
      KX(L) = KX(I)
      KX(I) = J
  100 IF (Q - EPS)   110, 110, 120
  110 KERR = 1
      RETURN
  120 KI = KX(I)
      Q = A(I, KI)
      IF (N - I)   150, 150, 130
  130 DO 140   J = IP1, N
      KJ = KX(J)
  140 A(I, KJ) = A(I, KJ) / Q
  150 CONTINUE
  160 DO 200   I = 1, N
      Q = B(I)
      IM1 = I - 1
      IF (IM1)   190, 190, 170
  170 DO 180   J = 1, IM1
      KJ = KX(J)
  180 Q = Q - A(I, KJ) * B(J)
  190 KI = KX(I)
  200 B(I) = Q / A(I, KI)
      DO 230   IC = 1, N
      I = N - IC + 1
      Q = B(I)
      IF (N - I)   230, 230, 210
  210 IP1 = I + 1
      DO 220   J = IP1, N
      KJ = KX(J)
  220 Q = Q - T(J) * A(I, KJ)
  230 T(I) = Q
      DO 240   J = 1, N
```

```
      KJ = KX(J)
  240 B(KJ) = T(J)
      RETURN
      END

      SUBROUTINE CALC (T,HOFJ,CP,S,H)

      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /COEFS /B(9)

      TH = T / 1000.0
      TH2 = TH * TH
      TH3 = TH2 * TH
      RTH = 1.0 / TH
      RTH2 = RTH * RTH
      RTH3 = RTH2 * RTH
      CP =(B(1) + B(2)*TH + B(3)*TH2 + B(4)*TH3 + B(5)*RTH + B(6)*RTH2
     $  + B(7)*RTH3)* 8.31451
      X = DLOG(TH)
      S = 8.31451 * ( B(1)*X  + B(2)*TH + B(3)*TH2/2.0 + B(4)*TH3/3.0
     $  - B(5)*RTH - B(6)*RTH2/2.0 - B(7)*RTH3/3.0 )  +  B(9)
      H = ( T * 8.31451 * ( B(1) + B(2)*TH/2.0 +  B(3)*TH2/3.0 +
     $   B(4)*TH3/4.0 + B(5)*RTH*X - B(6)*RTH2 - B(7)*RTH3/2.0)
     $   + B(8) -  HOFJ )
C     UU = ((H * 1000.0 + HOFJ) / T - S) / 8.31451
      RETURN
      END

      SUBROUTINE FMATR (IOPT, TEM, CP)
      IMPLICIT REAL*8 (A-H,O-Z)

      COMMON /LSTSQ/ T, T2, T3, T4, T5, T6, TM2, TM3, TM4, TM5, TM6,
     $  Y, YT2, YT3, TM, SN, YTM2, YT, YTM, YTM3

      IF (IOPT .NE. 0) GOTO 10
      Y = 0.0
      YT = 0.0
      YT2 = 0.0
      YT3 = 0.0
      YTM = 0.0
      YTM2 = 0.0
      YTM3 = 0.0
      SN = 0.0
      T = 0.0
      T2 = 0.0
      T3 = 0.0
      T4 = 0.0
      T5 = 0.0
      T6 = 0.0
```

```
      TM = 0.0
      TM2 = 0.0
      TM3 = 0.0
      TM4 = 0.0
      TM5 = 0.0
      TM6 = 0.0
      GOTO 20
   10 X = CP / 8.31451

C  CHECK print
C       WRITE (4, 9999) TEM, CP, T, X, Y
C9999  FORMAT (' TEM & Cp = ', 2F10.2, 3F15.4)

      TH = TEM / 1000.0
      TH2 = TH * TH
      TH3 = TH * TH2
      RTH = 1.0 / TH
      RTH2 = RTH * RTH
      RTH3 = RTH * RTH2
      Y = Y + X
      YT = YT + X * TH
      YT2 = YT2 + X * TH2
      YT3 = YT3 + X * TH3
      YTM = YTM + X * RTH
      YTM2 = YTM2 + X * RTH2
      YTM3 = YTM3 + X * RTH3
      SN = SN + 1.0
      T = T + TH
      T2 = T2 + TH2
      T3 = T3 + TH3
      T4 = T4 +  TH2 * TH2
      T5 = T5 +  TH2 * TH3
      T6 = T6 +  TH3 * TH3
      TM = TM + RTH
      TM2 = TM2 + RTH2
      TM3 = TM3 + RTH3
      TM4 = TM4 + RTH2 * RTH2
      TM5 = TM5 + RTH2 * RTH3
      TM6 = TM6 + RTH3 * RTH3
   20 RETURN
      END
```

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Appendix L.

Listing of Program TIGFIT5X

```
      PROGRAM TIGFIT5X

C
C  This version: 26 January 1993

C  Specifically adapted to creating coefficients for EXBLAKE.  This
C  program is the fourth of a series of programs named either TIGFITi
C  or TIGFIT1X (i = 1,4).  This program is specifically designed to
C  get its input from tables created by expanding the extended-range
C  fitting coefficients given to ARL/WTD/APCB by Ms. Bonnie McBride
C  (NASA Lewis Research Center).  The expansion was done by Program
C  EXCALCTH4 (q.v.).

C  This program has all of the features of its predecessors (use of the
C  '$' sentinel; computation of measures of goodness-of-fit); but it
C  does not include the cut-off at 15 000 K.

C  In this version, the output files have been changed from TIGFIT.OUT
C  and TIGFIT.AUX to TIGFIT5X.OUT and TIGFIT5X.AUX.

C  This one has all of the features of its predecessors (use of the '$'
C  sentinel; computation of measures of goodness-of-fit); but it does
C  not include the cut-off at 15 000 K.

C  For further important details, see the Comment lines at the beginning
C  of TIGFIT4X.

      IMPLICIT REAL*8 (A-H,O-Z)
C
      DIMENSION A(7,7), B(9), KX(7)
      DIMENSION TK(500), CPP(500), SS(500), HH(500)

      CHARACTER XNAME*10, PHASE*6, SENT*1
      PARAMETER (N6=0)
      LOGICAL HITEMP

      COMMON /COEFS/ B, NUM, NNUM
      COMMON /FUNCS/ TK, CPP, SS, HH, TFIX, TSTART, ENTRP0, HOFJ,
     $ XNAME, PHASE
      COMMON /IOSTUF/ LI, LO
      COMMON /LSTSQ/ T, T2, T3, T4, T5, T6, TM2, TM3, TM4, TM5, TM6,
     $  Y, YT2, YT3, TM, SN, YTM2, YT, YTM, YTM3

      DATA PHASE/ 'GAS   ' /
C
```

```
      LO = 6
      LI = 5
        OPEN (LI,FILE='TEMPS.IN',STATUS='OLD')
        OPEN (3,FILE='TIGFIT5X.OUT',STATUS='UNKNOWN')
        OPEN (LO,FILE='TIGFIT5X.AUX',STATUS='UNKNOWN')
        OPEN (4,FILE='CHEKK5X',STATUS='UNKNOWN')
        OPEN (2,FILE='CALORIC',ACCESS='APPEND',STATUS='UNKNOWN')
        WRITE (2, 81)
   81 FORMAT (' The data cards for the TIGER code are (units = calories'
     $ ', mols, & K): ')
C
C       CALL LOGO
C
      REWIND LI
      READ (LI, *, END=33) TFIX, TSTART
      CLOSE (LI)
      OPEN (LI,FILE='EXCALCTH.OUT',STATUS='OLD')
      REWIND LI
   10 READ(LI,1020,END=33) SENT, XNAME
 1020 FORMAT(A1, A10 )
      IF (SENT .NE. '$') GOTO 10

        WRITE (N6,2008) XNAME
 2008   FORMAT(1X,'Processing ==> ',A10)
C  Initialize the elements that will make up the matrix
      CALL FMATR (0, X1, X2)

C  Read the first line of data.
   15 READ(LI,*, END=33) TEM, CP, ENTRP0, HMH298, HOFJ
C     WRITE (LO,*) "Input 1", TEM, CP, ENTROP, HMH298, HOFJ
C  Is temperature the pinning temperature? If not, read another line.
      IF (TEM. LT. TFIX-0.05 .OR. TEM .GT. TFIX+0.05 ) GOTO 15
C  Yes, it is the pinning T.  Is T Fix = T Start?
C  If it is, then start saving data and continue to read the table
   20 IF (TEM .GE. TSTART-0.05 .AND. TEM .LE. TSTART+0.05 ) THEN
                KT = 1
                TK(1) = TSTART
                CPP(1) = CP
                SS(1) = ENTRP0
                HH(1) = HMH298
                GOTO 35
      END IF
C  No, T Fix wasn't T Start.  Keep looking for T Start
   25 READ (LI,*, END=33, ERR=999) TEM, CP, ENTROP, HMH298, ENTHALP
C     WRITE (LO,*) "Input2", TEM, CP, ENTROP, HMH298, ENTHALP
      IF (TEM .LT. TSTART-0.05 .OR . TEM .GT. TSTART+0.05 ) GOTO 25
C  At last T Start has been found; save values and keep reading table.
   29 KT = 1
      TK(1) = TSTART
```

```
      CPP(1) = CP
      SS(1) = ENTROP
      HH(1) = HMH298
      HITEMP = .FALSE.

      CALL FMATR (1, TK(1), CP)
   35 KT = KT + 1
      READ(LI,*, END=33) TEM, CP,ENTROP, HMH298, ENTHALP
C     WRITE (LO, *) "Input3", TEM, CP,ENTROP, HMH298, ENTHALP
      TK(KT) = TEM
      CPP(KT) = CP
      SS(KT) = ENTROP
      HH(KT) = HMH298
C        WRITE (LO,*) TEM, CP, ENTROP
      IF (TEM .LE. 14999.) GOTO 49
      IF (TEM .EQ. 15000.) THEN
         HITEMP = .TRUE.
         GOTO 60
      END IF

   49 IF (CP .EQ. 999.0)  GOTO 60
      CALL FMATR (1, TK(KT), CP)
      IF (.NOT. HITEMP) GOTO 35
C  The end of the table has been reached.  Is the last temperature
C  equal to or greater than 10 000 K?
   60 NUM=KT-1

      IF (HITEMP) NUM=KT

      IF (TK(NUM) .GE. 1.D4) THEN
            NNUM=0
            GOTO 61
      END IF
   61 CALL EXTEND (TK, CPP, NUM, NNUM)
      B(1) = Y
      B(2) = YT
      B(3) = YT2
      B(4) = YT3
      B(5) = YTM
      B(6) = YTM2
      B(7) = YTM3
      A(1,1) = SN
      A(2,5) = SN
      A(3,6) = SN
      A(4,7) = SN
      A(5,2) = SN
      A(6,3) = SN
      A(7,4) = SN
      A(2,1) = T
```

```
      A(3,5) = T
      A(4,6) = T
      A(1,2) = T
      A(5,3) = T
      A(6,4) = T
      A(3,1) = T2
      A(2,2) = T2
      A(4,5) = T2
      A(1,3) = T2
      A(5,4) = T2
      A(4,1) = T3
      A(2,3) = T3
      A(1,4) = T3
      A(3,2) = T3
      A(5,1) = TM
      A(2,6) = TM
      A(3,7) = TM
      A(1,5) = TM
      A(6,2) = TM
      A(7,3) = TM
      A(6,1) = TM2
      A(2,7) = TM2
      A(5,5) = TM2
      A(1,6) = TM2
      A(7,2) = TM2
      A(7,1) = TM3
      A(5,6) = TM3
      A(1,7) = TM3
      A(6,5) = TM3
      A(2,4) = T4
      A(3,3) = T4
      A(4,2) = T4
      A(3,4) = T5
      A(4,3) = T5
      A(4,4) = T6
      A(5,7) = TM4
      A(6,6) = TM4
      A(7,5) = TM4
      A(6,7) = TM5
      A(7,6) = TM5
      A(7,7) = TM6
      CALL SOLVEX(7, A, B, KX, 0, KERR)
      IF (KERR .LE. 0)  GOTO 66
   64 STOP
   66 X= TFIX/1000.
      B(8)  =  HOFJ - TFIX * 8.31451 * ( ( ( B(4) * X / 4.0  + B(3)/
     A 3.0 ) * X  +  B(2) / 2.0 ) * X  + B(1) - ( ( B(7) / (X * 2.0)
     A + B(6)) / X  - B(5) * DLOG(X) ) / X )
      B(9)  = ENTRP0 - 8.31451 * ( ( ( B(4) * X / 3.0 + B(3) / 2.0 )
```

```
     A * X + B(2) ) * X  + B(1) * DLOG(X) - ( ( B(7) / (3.0 * X) +
     A B(6) / 2.0 ) / X  + B(5) ) / X )

      WRITE (LO, 70)  XNAME, PHASE
   70 FORMAT(5X, A10, /, 5X, 13HThe phase is , A6, / )

      WRITE (LO,22) TFIX, TSTART, ENTRP0, HOFJ
   22 FORMAT (' Fit fixed at T    =', F11.2/
     $        ' Fit starts at T   =', F11.2/
     $        ' Entropy at T Fix  =', F11.2/
     $        ' Enthalpy at T Fix =', F10.1 / )

C ***********************************************
C     WRITE (4, 71)  XNAME, PHASE
C  71 FORMAT(/5X, A10, 'Phase = ', A6/)

C     DO 9877 IJK=1,NUM,4
C     IJK1 = IJK
C     IJK2 = IJK1+3
C     IF (IJK2 .GT. NUM) IJK2 = NUM
C9877 WRITE (4, 9878) (IJ, TK(IJ), IJ=IJK1,IJK2)
C9878 FORMAT (4(I5,')',F8.1,3X))
C ***********************************************************

      WRITE (LO, 80)
   80 FORMAT (' The data cards for the TIGER code are (units = Joules, '
     $ ' mols, & K): '/)
      I = 1
      WRITE (LO,90)  XNAME, PHASE, I, B(1), B(2), B(3)
      WRITE (3, 95)  XNAME, PHASE, I, B(1), B(2), B(3)
      WRITE (2, 95)  XNAME, PHASE, I, B(1), B(2), B(3)
      I = 2
      WRITE (LO,90)  XNAME, PHASE, I, B(4), B(5), B(6)
      WRITE (3, 95)  XNAME, PHASE, I, B(4), B(5), B(6)
      WRITE (2, 95)  XNAME, PHASE, I, B(4), B(5), B(6)
      I = 3
      WRITE (LO,90)  XNAME, PHASE, I, B(7), B(8), B(9)
      WRITE (3, 95)  XNAME, PHASE, I, B(7), B(8), B(9)
      B8 = B(8)/4.184D0
      B9 = B(9)/4.184D0
      WRITE (2, 95)  XNAME, PHASE, I, B(7), B8, B9
   90 FORMAT(2X, 5HSTR, , A6, ',', A6, ',' ,I1,3(2H, ,1PD15.7))
   95 FORMAT(     5HSTR, , A6, ',', A6, ',', I1,3(2H, ,1PD15.7))

C     WRITE (4, 110)
  110 FORMAT(/'      T          CP          S          '
     $ 'H-H298       MU/RT')
  120 FORMAT(1X,F8.2,F15.3,F15.3,F14.3,F14.4)
```

```
      T = 298.15
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120)  T, CP, S, H
      T = 300.0
      DO  130  I = 1, 18
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120) T, CP, S, H, UU
  130 T = T + 100.0
C     WRITE (LO, 70)  XNAME, PHASE
C     WRITE (LO, 110)
      DO 140  I = 1, 30
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120) T, CP, S, H, UU
  140 T = T + 100.0
C     GOTO 10
      T = 6000.0
      DO 150  I = 1,9
      CALL CALC (T,HOFJ,CP,S,H)
C     WRITE (4, 120) T, CP, S, H, UU
  150 T = T + 1000.0
      CALL GOODF5X
      GO TO 10

  999 WRITE (LO, *) TEM, CP, X1, HMH298, ENTROP, X2
      WRITE (4, *) TEM, CP, X1, HMH298, ENTROP, X2
   33 STOP
      END

      SUBROUTINE CALC (T,HOFJ,CP,S,H)

      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /COEFS /B(9)

      TH = T / 1000.0
      TH2 = TH * TH
      TH3 = TH2 * TH
      RTH = 1.0 / TH
      RTH2 = RTH * RTH
      RTH3 = RTH2 * RTH
      CP =(B(1) + B(2)*TH + B(3)*TH2 + B(4)*TH3 + B(5)*RTH + B(6)*RTH2
     $  + B(7)*RTH3)* 8.31451
      X = DLOG(TH)
      S = 8.31451 * ( B(1)*X  + B(2)*TH + B(3)*TH2/2.0 + B(4)*TH3/3.0
     $  - B(5)*RTH - B(6)*RTH2/2.0 - B(7)*RTH3/3.0 )  +  B(9)
      H = ( T * 8.31451 * ( B(1) + B(2)*TH/2.0 +  B(3)*TH2/3.0 +
     $   B(4)*TH3/4.0 + B(5)*RTH*X - B(6)*RTH2 - B(7)*RTH3/2.0)
     $   + B(8) -  HOFJ )
      RETURN
      END
```

```
      SUBROUTINE FMATR (IOPT, TEM, CP)
      IMPLICIT REAL*8 (A-H,O-Z)

      COMMON /LSTSQ/ T, T2, T3, T4, T5, T6, TM2, TM3, TM4, TM5, TM6,
     $  Y, YT2, YT3, TM, SN, YTM2, YT, YTM, YTM3

      IF (IOPT .NE. 0) GOTO 10
      Y = 0.0
      YT = 0.0
      YT2 = 0.0
      YT3 = 0.0
      YTM = 0.0
      YTM2 = 0.0
      YTM3 = 0.0
      SN = 0.0
      T = 0.0
      T2 = 0.0
      T3 = 0.0
      T4 = 0.0
      T5 = 0.0
      T6 = 0.0
      TM = 0.0
      TM2 = 0.0
      TM3 = 0.0
      TM4 = 0.0
      TM5 = 0.0
      TM6 = 0.0
      GOTO 20
   10 X = CP / 8.31451

C  CHECK print
C       WRITE (4, 9999) TEM, CP, T, X, Y
C9999  FORMAT (' TEM & Cp = ', 2F10.2, 3F15.4)

      TH = TEM / 1000.0
      TH2 = TH * TH
      TH3 = TH * TH2
      RTH = 1.0 / TH
      RTH2 = RTH * RTH
      RTH3 = RTH * RTH2
      Y = Y + X
      YT = YT + X * TH
      YT2 = YT2 + X * TH2
      YT3 = YT3 + X * TH3
      YTM = YTM + X * RTH
      YTM2 = YTM2 + X * RTH2
      YTM3 = YTM3 + X * RTH3
      SN = SN + 1.0
      T = T + TH
```

```
      T2 = T2 + TH2
      T3 = T3 + TH3
      T4 = T4 +  TH2 * TH2
      T5 = T5 +  TH2 * TH3
      T6 = T6 +  TH3 * TH3
      TM = TM + RTH
      TM2 = TM2 + RTH2
      TM3 = TM3 + RTH3
      TM4 = TM4 + RTH2 * RTH2
      TM5 = TM5 + RTH2 * RTH3
      TM6 = TM6 + RTH3 * RTH3
   20 RETURN
      END
      SUBROUTINE SOLVEX(N, A, B, KX, K, KERR)
C
        IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(7,7), B(9), KX(7), T(7)
      EPS = 0.0
      KERR = 0
      IF (K)  10, 10, 160
   10 DO 20  J = 1, N
   20 KX(J) = J
      DO 150  I = 1, N
      IM1 = I - 1
      IF (IM1)  50, 50, 30
   30 DO 40  J = 1, IM1
      KJ = KX(J)
      Q = A(I, KJ)
      JP1 = J + 1
      DO 40  L = JP1, N
      KL = KX(L)
   40 A(I, KL) = A(I, KL) - Q * A(J, KL)
   50 KI = KX(I)
      Q = DABS(A(I, KI))
      IF (N - I)  100, 100, 60
   60 L = I
      IP1 = I + 1
      DO 80  J = IP1, N
      KJ = KX(J)
      AIKJ = DABS(A(I, KJ))
      IF (AIKJ - Q)  80, 80, 70
   70 Q = AIKJ
      L = J
   80 CONTINUE
      IF (L - I)  90, 100, 90
   90 J = KX(L)
      KX(L) = KX(I)
      KX(I) = J
  100 IF (Q - EPS)  110, 110, 120
```

```
110 KERR = 1
    RETURN
120 KI = KX(I)
    Q = A(I, KI)
    IF (N - I)  150, 150, 130
130 DO 140  J = IP1, N
    KJ = KX(J)
140 A(I, KJ) = A(I, KJ) / Q
150 CONTINUE
160 DO 200  I = 1, N
    Q = B(I)
    IM1 = I - 1
    IF (IM1)  190, 190, 170
170 DO 180  J = 1, IM1
    KJ = KX(J)
180 Q = Q - A(I, KJ) * B(J)
190 KI = KX(I)
200 B(I) = Q / A(I, KI)
    DO 230  IC = 1, N
    I = N - IC + 1
    Q = B(I)
    IF (N - I)  230, 230, 210
210 IP1 = I + 1
    DO 220  J = IP1, N
    KJ = KX(J)
220 Q = Q - T(J) * A(I, KJ)
230 T(I) = Q
    DO 240  J = 1, N
    KJ = KX(J)
240 B(KJ) = T(J)
    RETURN
    END
```

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